Concrete Mixture Optimization Using Statistical Methods: Final Report

PUBLICATION NO. FHWA-RD-03-060

SEPTEMBER 2003

U.S. Department of Transportation
Federal Highway Administration

FOREWORD

This report presents the results of a study conducted jointly by the Federal Highway Administration and the National Institute of Standards and Technology to assess the feasibility of using statistical experiment design and analysis methods to optimize concrete mixture proportions. The laboratory phase of the study indicated that both the classical mixture method and the factorial approach could be applied to the problem of optimizing concrete mixture proportions. The factorial approach was used as the basis for developing an Internet-based computer program, the Concrete Optimization Software Tool, in the second phase of this project. This tool, accessible on the Web, allows a potential user to learn about and try this statistical approach. This report will be of interest to materials engineers and others who are involved in concrete construction and concrete mixture design, materials selection, and proportioning.

T. Paul Teng
T. Paul Teng, P.E.
Director, Office of Infrastructure
Research and Development

NOTICE

Technical Report Documentation Page

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
FHWA-RD-03-060		

4. Title and Subtitle Concrete Mixture Optimization Using Statistical Methods: Final Report	5. Report Date September 2003 6. Performing Organization Code 480017
7. Author(s) M.J. Simon	8. Performing Organization Report No.
9. Performing Organization Name and Address FHWA Office of Infrastructure Research and Development, 6300 Georgetown Pike, McLean, VA 22101 National Institute of Standards and Technology, Building Materials Division, 100 Bureau Drive, Gaithersburg, MD 20899 National Institute of Standards and Technology, Statistical Engineering Division, 100 Bureau Drive, Gaithersburg, MD 20899	10. Work Unit No. 11. Contract or Grant No. **DTFH61-97-Y-30033**
12. Sponsoring Agency Name and Address Office of Infrastructure Research and Development Federal Highway Administration 6300 Georgetown Pike McLean, VA 22101-2296	13. Type of Report and Period Covered Final Report November, 1996 to July, 2003 14. Sponsoring Agency Code

15. Supplementary Notes

This project was a cooperative effort between the FWHA Office of Infrastructure Research and Development, the NIST Building and Fire Reseach Laboratory (Building Materials Division), and the NIST Information Technology Laboratory (Statistical Engineering Division).

16. Abstract

This report presents the results of a research project whose goals were to investigate the feasibility of using statistical experiment design and analysis methods to optimize concrete mixture proportions and to develop an Internet-based software program to optimize concrete mixtures using these methods. Two experiment design approaches (classical mixture and factorial-based central composite design) were investigated in laboratory experiments. In each case, six component materials were used, and mixtures were optimized for four performance criteria (properties) and cost. Based on the experimental results, the factorial-based approach was selected as the basis for the Internet-based system. This system, the Concrete Optimization Software Tool (COST), employs a six-step interactive procedure starting with materials selection and working through trial batches, testing, and analysis of test results. The end result is recommended mixture proportions to achieve the desired performance levels. COST was developed as a tool to introduce the industry to the potential benefits of using statistical methods in concrete mixture proportioning, and to give interested parties an opportunity to try the methods for themselves.

17. Key Words	18. Distribution Statement
Building technology, pavements, structures, concrete, mixture proportioning, experiment design, optimization, response surface methods	No restrictions. This document is available to the public through the National Technical Information Service, Springfield, VA 22161.

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No of Pages	22. Price
Unclassified	Unclassified	167	

Form DOT F 1700.7 (8-72) **Reproduction of completed pages authorized**

SI* (MODERN METRIC) CONVERSION FACTORS

APPROXIMATE CONVERSIONS TO SI UNITS

Symbol	When You Know	Multiply By	To Find	Symbol
		LENGTH		
in	inches	25.4	millimeters	mm
ft	feet	0.305	meters	m
yd	yards	0.914	meters	m
mi	miles	1.61	kilometers	km
		AREA		
in^2	square inches	645.2	square millimeters	mm^2
ft^2	square feet	0.093	square meters	m^2
yd^2	square yard	0.836	square meters	m^2
ac	acres	0.405	hectares	ha
mi^2	square miles	2.59	square kilometers	km^2
		VOLUME		
fl oz	fluid ounces	29.57	milliliters	mL
gal	gallons	3.785	liters	L
ft^3	cubic feet	0.028	cubic meters	m^3
yd^3	cubic yards	0.765	cubic meters	m^3
	NOTE: volumes greater than 1000 L shall be shown in m^3			
		MASS		
oz	ounces	28.35	grams	g
lb	pounds	0.454	kilograms	kg
T	short tons (2000 lb)	0.907	megagrams (or "metric ton")	Mg (or "t")
		TEMPERATURE (exact degrees)		
°F	Fahrenheit	5 (F-32)/9 or (F-32)/1.8	Celsius	°C
		ILLUMINATION		
fc	foot-candles	10.76	lux	lx
fl	foot-Lamberts	3.426	candela/m^2	cd/m^2
		FORCE and PRESSURE or STRESS		
lbf	poundforce	4.45	newtons	N
lbf/in^2	poundforce per square inch	6.89	kilopascals	kPa

APPROXIMATE CONVERSIONS FROM SI UNITS

Symbol	When You Know	Multiply By	To Find	Symbol
		LENGTH		
mm	millimeters	0.039	inches	in
m	meters	3.28	feet	ft
m	meters	1.09	yards	yd
km	kilometers	0.621	miles	mi
		AREA		
mm^2	square millimeters	0.0016	square inches	in^2
m^2	square meters	10.764	square feet	ft^2
m^2	square meters	1.195	square yards	yd^2
ha	hectares	2.47	acres	ac
km^2	square kilometers	0.386	square miles	mi^2
		VOLUME		
mL	milliliters	0.034	fluid ounces	fl oz
L	liters	0.264	gallons	gal
m^3	cubic meters	35.314	cubic feet	ft^3
m^3	cubic meters	1.307	cubic yards	yd^3
		MASS		
g	grams	0.035	ounces	oz
kg	kilograms	2.202	pounds	lb
Mg (or "t")	megagrams (or "metric ton")	1.103	short tons (2000 lb)	T
		TEMPERATURE (exact degrees)		
°C	Celsius	1.8C+32	Fahrenheit	°F
		ILLUMINATION		
lx	lux	0.0929	foot-candles	fc
cd/m^2	candela/m^2	0.2919	foot-Lamberts	fl
		FORCE and PRESSURE or STRESS		
N	newtons	0.225	poundforce	lbf
kPa	kilopascals	0.145	poundforce per square inch	lbf/in^2

*SI is the symbol for the International System of Units. Appropriate rounding should be made to comply with Section 4 of ASTM E380.
(Revised March 2003)

TABLE OF CONTENTS

TABLE OF CONTENTS (continued)

LIST OF FIGURES

LIST OF FIGURES (continued)

LIST OF FIGURES (continued)

Figure | Page

LIST OF FIGURES (continued)

LIST OF TABLES

LIST OF TABLES (continued)

CHAPTER 1
Introduction

1.1 Statement of Problem and Project Goals

The purpose of this project was to investigate the use of statistical experiment design approaches in concrete mixture proportioning. These statistical methods are applied in industry to optimize products such as gasoline, food products, and detergents. In many cases, the products are, like concrete, combinations of several components. Typically, these applications optimize a product to meet a number of performance criteria (user-specified constraints) simultaneously, at minimum cost. For concrete, these performance criteria could include fresh concrete properties such as viscosity, yield stress, setting time, and temperature; mechanical properties such as strength, modulus of elasticity, creep, and shrinkage; and durability-related properties such as resistance to freezing and thawing, abrasion, or chloride penetration.

This project was sponsored by the Federal Highway Administration (FHWA) and was performed jointly by researchers from FHWA and the National Institute of Standards and Technology (NIST) Building Materials and Statistical Engineering Divisions. Both FHWA and NIST hope to facilitate the use of high-performance concrete (HPC) in both public and private construction, and are currently working to develop tools for optimizing HPC mixture proportions.

HPC has been referred to as "engineered concrete," implying that an HPC mixture is not specified in a generic recipe, but rather designed to meet project-specific needs [1]. Such a definition gives a concrete producer or materials engineer greater than usual latitude in selecting constituent materials and defining proportions in an HPC mixture, since fewer or possibly no prescriptive constraints, such as minimum cement contents or maximum water-cement (w/c) ratios, are included in specifications. HPC mixtures are usually more expensive than conventional concrete mixtures because they usually contain more cement, several chemical admixtures at higher dosage rates than for conventional concrete, and one or more supplementary cementitious materials. As the cost of materials increases, optimizing concrete mixture proportions for cost becomes more desirable. Furthermore, as the number of constituent materials increases, the problem of identifying optimal mixtures becomes increasingly complex. Not only are there more materials to consider, but there also are more potential interactions among materials. Combined with several performance criteria, the number of trial batches required to find optimal proportions using traditional methods could become prohibitive.

The general approach to concrete mixture proportioning can be described by the following steps:

1. Identifying a starting set of mixture proportions.

2. Performing one or more trial batches, starting with the mixture identified in step 1 above, and adjusting the proportions in subsequent trial batches until all criteria are satisfied.

Current practice in the United States for developing new concrete mixtures often relies upon using historical information (i.e., what has worked for the producer in the past) or guidelines for mixture proportioning outlined in American Concrete Institute (ACI) 211.1 [2]. Following the ACI 211.1 guidelines, an engineer would select and run a first trial batch (selecting proportions using ACI 211.1 or historical data), evaluate the results, adjust the proportions of various components, and run further trial batches until all specified criteria are met. Typically, this is performed by varying one component at a time. While both historical information and ACI 211.1 can yield a starting point for trial batches, neither method is a comprehensive procedure for optimizing mixtures. Historical information may not be valid for materials other than the particular ones used in a given project. In ACI 211.1, interactions among the concrete constituents cannot be accounted for, and there is no means to achieve an efficiently optimized mixture for a given criterion.

In contrast, statistical experimental design methods are rigorous techniques for both achieving desired properties and determining an optimized mixture for a given set of constraints. They are used widely in industry to optimize products and processes [3], and have been applied in some research studies on improving high-performance concrete [4,5]. They have not, however, been applied as a general approach to concrete mixture proportioning.

Employing statistical methods in the trial batch process does not change the overall approach, but it changes the trial batch process. Rather than selecting one starting point, a set of trial batches covering a chosen range of proportions for each component is defined according to established statistical procedures [3]. Trial batches are then carried out, test specimens are fabricated and tested, and results are analyzed using standard statistical methods. These methods include fitting empirical models to the data for each performance criterion. In these models, each response (resultant concrete property) such as strength, slump, or cost, is expressed as an algebraic function of factors (individual component proportions) such as w/c, cement content, chemical admixture dosage, and percent pozzolan replacement.

After a response can be characterized by an equation (model), several analyses are possible. For instance, a user could determine which mixture proportions would yield one or more desired properties. A user also could optimize any property subject to constraints on other properties. Simultaneous optimization to meet several constraints is also possible. For example, one could determine the lowest cost mixture with strength greater than a specified value, air content within a given range, and slump within a given range. A method for optimizing several responses simultaneously is described later in the report.

Mechanistic (or semimechanistic) models that were developed from results of fundamental and applied materials research have also been used as a basis for mixture proportioning methods [6]. An advantage of this approach is that it does not require trial batches to obtain the models; however, some trial batches most likely would be needed to adjust proportions because of differences in material properties at the local level. It is unlikely that a mechanistic model would be able to account for all possible differences in local materials. The advantage of the trial batch approach is that the project-specific materials are used and accounted for in the model.

An additional advantage of the statistical approach is that the expected properties (responses) can be characterized by an uncertainty (variability). This has important implications for specifications and for production. When an empirical model equation is used to determine mixture proportions that yield a desired strength, the model equation gives only the expected mean strength; that is, if replicate mixtures were made, the model equation would predict the mean value. This is not an appropriate target value for specifications, because in the long run, the strength would be below that value half of the time. Instead, to ensure that most of the strength test results would comply with specifications, a producer would select target values for the mean strength to account for the variability and to ensure that, for example, 95 percent of the results would be expected to meet or exceed the specified value.

A disadvantage of the statistical approach is that it requires an initial investment of time and money for planning and performing trial batches and tests. Additionally, knowledge of good experimentation procedures and some knowledge of statistical analysis is needed. Statistical computer programs are available to perform both experiment design and analysis, but knowing how to interpret and ensure the validity of statistical models is important. For this reason, the second objective of this project was to develop an interactive Web site to provide users with rudimentary knowledge and lead them step by step through a mixture proportioning process using statistical methods. The aim was not to provide a comprehensive, user-friendly software package, but rather to introduce producers and engineers to these methods and to provide sufficient results and guidance on interpretation to allow them to see potential advantages of the approach.

Although these methods require a commitment of time and money upfront, they have the potential to save money during construction. Reducing the concrete material cost by $20 per cubic meter ($m^3$) could result in savings of $40,000 per km of 30-cm thick, two-lane concrete pavement.

1.2 Scope of Report

The report is organized as follows: Chapter 1 introduces the problem and the project goals, and describes the scope. Chapter 2 provides background on the statistical concepts used in this project, including response surface methodology (RSM) and its components: experiment design, model fitting and validation, and optimization. Chapter 3 describes the laboratory experiment using a mixture experiment design approach, and chapter 4 describes a laboratory experiment using a mathematically independent variable (MIV), or factorial, approach. Chapter 5 describes the development of the interactive Web site, the Concrete Optimization Software Tool (COST). References are provided after chapter 5. Appendices A (mixture experiment) and B (factorial experiment) contain experiment designs, test data, data analysis and model fitting (tables and graphs) from the laboratory experiments. Appendix C contains the COST User's Guide, which describes the COST system and its use in detail.

CHAPTER 2
Background on Statistical Methods

2.1 Response Surface Methodology

Response surface methodology (RSM) consists of a set of statistical methods that can be used to develop improve, or optimize products [3]. RSM typically is used in situations where several factors (in the case of concrete, the proportions of individual component materials) influence one or more performance characteristics, or responses (the fresh and hardened properties of the concrete). RSM may be used to optimize one or more responses (e.g., maximize strength, minimize chloride penetration), or to meet a given set of specifications (e.g., a minimum strength specification or an allowable range of slump values). There are three general steps that comprise RSM: experiment design, modeling, and optimization. Each of these is described below.

Concrete is a mixture of several components. Water, portland cement, and fine and coarse aggregates form a basic concrete mixture. Various chemical and mineral admixtures, as well as other materials such as fibers, also may be added. For a given set of materials, the proportions of the components directly influence the properties of the concrete mixture, both fresh and hardened.

2.2 Experiment Design

Consider a concrete mixture consisting of q component materials (where q is the number of component materials). Two experiment design approaches can be applied to concrete mixture optimization: the classic mixture approach, in which the q mixture components are the variables, [7] and the mathematically independent variable (MIV) approach, in which q mixture components are transformed into $q-1$ independent mixture-related variables [8]. Each technique has advantages and disadvantages. In the classic mixture approach, the sum of the proportions must be 1; therefore the variables are not all independent. This allows the experimental region of interest to be defined more naturally, but the analysis of such experiments is more complicated. The MIV approach, with the variables independent, permits the use of classical factorial and response surface designs [9], but has the undesirable feature that the experimental region changes depending on how the q mixture components are reduced to $q-1$ independent factors.

In this report, the MIV approach is referred to as the factorial approach because factorial experiment designs form the basis of the approach. The following sections present general (nonrigorous) descriptions of each method (for a detailed discussion of these methods, see reference 3).

2.2.1 Mixture Approach

In the mixture approach, the total amount (mass or volume) of the product is fixed, and the settings of each of the q components are proportions. Because the total amount is constrained to sum to one, only $q-1$ of the factors (component variables) can be chosen independently.

As a simple (hypothetical) example of a mixture experiment, consider concrete as a mixture of three components: water (x_1), cement (x_2), and aggregate (x_3), where each x_i represents the volume fraction of a component. Assume the coarse-to-fine aggregate ratio is held constant. The volume fractions of the components sum to one, and the region defined by this constraint is the regular triangle (or simplex) shown in figure 1. The axis for each component x_i extends from the vertex it labels ($x_i = 1$) to the midpoint of the opposite side of the triangle ($x_i = 0$). The vertex represents the pure component. For example, the vertex labeled x_1 is the pure water mixture with $x_1 = 1$, $x_2 = 0$, and $x_3 = 0$, or (1,0,0). The point where the three axes intersect, with coordinates (1/3,1/3,1/3), is called the centroid.

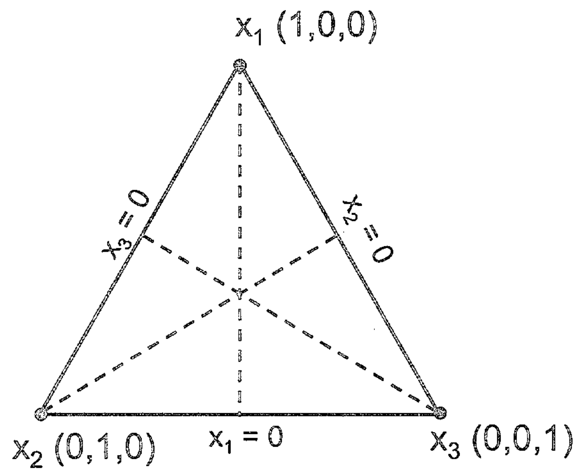


Figure 1. Example of triangular simplex region from three-component mixture experiment

A good experiment design for studying properties over the entire region of a three-component mixture would be the simplex-centroid design shown in figure 2 (this example is included as an illustration only, since much of this region would not represent either feasible or workable

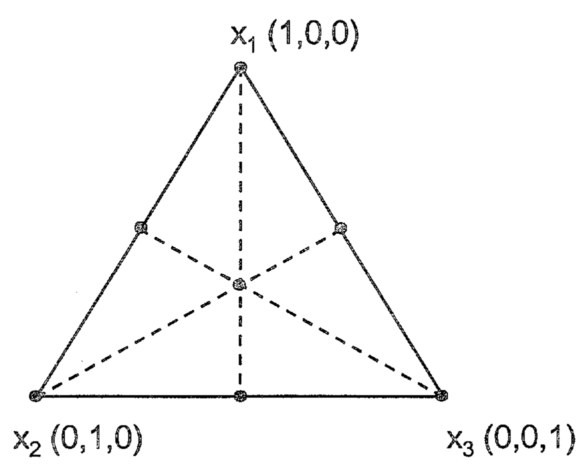


Figure 2. Simplex-centroid design for three variables

concrete mixtures). The points shown in figure 2 represent mixtures included in the experiment and include all vertices, midpoints of edges, and the overall centroid.

All responses (properties) of interest would be measured for each mixture in the design and modeled as a function of the components. Typically, polynomial functions are used for modeling, but other functional forms can also be used. For three components, the linear polynomial model for a response y is:

$$y = b_0^* + b_1^* x_1 + b_2^* x_2 + b_3^* x_3 + e \qquad (1)$$

where the b_i * are constants and e, the random error term, represents the combined effects of all variables not included in the model. For a mixture experiment, $x_1 + x_2 + x_3 = 1$; therefore, the model can be reparameterized in the form:

$$y = b_1 x_1 + b_2 x_2 + b_3 x_3 + e \qquad (2)$$

using $b_0^* = b_0^* \cdot (x_1 + x_2 + x_3)$. This form is called the Scheffé linear mixture polynomial [7].

Similarly, the quadratic polynomial:

(3)

$$y = b_0 + b_1^* x_1 + b_2^* x_2 + b_3^* x_3 + b_{12}^* x_1 x_2 + b_{13}^* x_1 x_3 + b_{23}^* x_2 x_3 + b_{11}^* x_1^2 + b_{22}^* x_2^2 + b_{33}^* x_3^2 + e \qquad (4)$$

can be reparameterized as:

$$y = b_1 x_1 + b_2 x_2 + b_3 x_3 + b_{12} x_1 x_2 + b_{13} x_1 x_3 + b_{23} x_2 x_3 + e$$

using $x_1^2 = x_1 \cdot (1 - x_2 - x_3)$, $x_2^2 = x_2 \cdot (1 - x_1 - x_3)$, and $x_3^2 = x_3 \cdot (1 - x_1 - x_2)$.

Since feasible concrete mixtures do not exist over the entire region shown in figures 1 and 2, a subregion of the full simplex containing the range of feasible mixtures must be defined by constraining the component proportions. An example of a possible subregion for the three-component example is shown in figure 3. It is defined by the following volume fraction constraints (where x_1 = water, x_2 = cement, x_3 = aggregate):

$$0.15 \leq x_1 \leq 0.25$$
$$0.10 \leq x_2 \leq 0.20$$
$$0.60 \leq x_3 \leq 0.70$$

In this case the simplex designs are usually no longer appropriate and other designs are used [3].

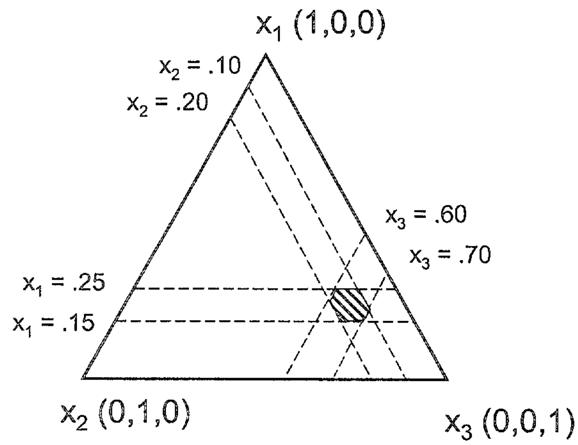


Figure 3. Example of subregion of full simplex containing range of feasible mixtures

The advantage of the mixture approach is that the experimental region of interest is defined more naturally; however, analysis of the results can be complicated, especially if the number of components is greater than three.

2.2.2 Factorial (MIV) Approach

In the factorial approach, the q components of a mixture are reduced to $q-1$ independent variables using the ratio of two components as an independent variable. In the case of concrete, w/c is a natural choice for this ratio variable. For the situation with $q-1$ independent variables, a 2^{q-1} factorial design forms the backbone of the experiment. This design consists of several factors (variables) set at two different levels. As a simple example, consider a concrete mixture composed of four components: water, cement, fine aggregate, and coarse aggregate. Three independent factors, or variables, x_k, that can be selected to describe this system are x_1 = w/c (by mass), x_2 = fine aggregate volume fraction, and x_3 = coarse aggregate volume fraction. Reasonable ranges for these variables might be:

$$0.40 \leq x_1 \leq 0.50$$
$$0.25 \leq x_2 \leq 0.30$$
$$0.40 \leq x_3 \leq 0.45$$

The levels for this example would be 0.40 and 0.50 for x_1, 0.25 and 0.30 for x_2, and 0.40 and 0.45 for x_3. To simplify calculations and analysis, the actual variable ranges are usually transformed to dimensionless coded variables with a range of ±1. In this example, the actual range of $0.40 \leq x_1 \leq 0.50$ would translate to a coded range of $-1 \leq x_1 \leq 1$. Intermediate values of x_1 would translate similarly (e.g., the actual value of 0.45 would translate to a coded value of zero). The general equation used to translate from coded to uncoded is as follows:

$$x_{actual} = x_{\min} + \frac{(x_{coded} + 1)}{2} \cdot (x_{\max} - x_{\min}) \qquad (5)$$

where x_{actual} is the uncoded value, x_{min} and x_{max} are the uncoded minimum and maximum values (corresponding to −1 and +1 coded values), and x_{coded} is the coded value to be translated.

Suppose that the specifications for this mixture require a slump of 75 to 150 mm and a 28-day strength of 30 MPa. These specified properties are called the responses, or dependent variables, y_i, which are the performance criteria for optimizing the mixture. For concrete, the responses may be any measurable plastic or hardened properties of the mixture. Cost may also be a response.

As with the mixture approach, empirical models are fit to the data, and polynomial models (linear or quadratic) typically are used. Equation 6 illustrates the general case of the full quadratic model for k =3 independent variables:

$$y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3 + b_{12} x_1 x_2 + b_{13} x_1 x_3 + b_{23} x_2 x_3 + b_{11} x_1^2 + b_{22} x_2^2 + b_{33} x_3^2 + e \qquad (6)$$

In equation 6, the ten coefficients are represented by the b_k and e is a random error term representing the combined effects of variables not included in the model. The interaction terms ($x_i x_j$) and the quadratic terms (x_i^2) account for curvature in the response surface.

The central composite design (CCD), an augmented factorial design, is commonly used in product optimization. A complete CCD experiment design allows estimation of a full quadratic model for each response. A schematic layout of a CCD for k = 3 independent variables is shown in figure 4. The design consists of 2^k (in this case, 8) factorial points (filled circles in figure 4) representing all combinations of coded values $x_k = \pm 1$, $2*k$ (in this case, 6) axial points (hollow circles in figure 4) at a distance $\pm\alpha$ from the origin, and at least 3 center points (hatched circle in figure 4) with coded values of zero for each x_k. The value of α usually is chosen to make the design rotatable[1], but there are sometimes valid reasons to select other values [3].

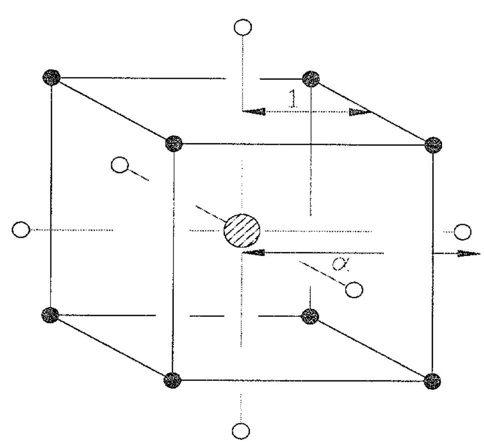


Figure 4. Schematic of a central composite design for three factors

[1]If a design is rotatable, predicted values should have equal variances at locations equidistant from the origin.

In the absence of curvature, a model with only linear terms would be sufficient, and the factorial portion of the CCD is a valid design by itself in that case. However, the presence or absence of significant curvature often is not known with certainty at the start. An advantage of the CCD over the mixture approach is that the CCD can be run sequentially in two blocks. The first block would consist of the factorial points (all combinations of $x_i = \pm 1$) and some center points (at least 3), and the second block would consist of the axial points (points along each axis at distance α from the origin) and additional center points (at least 2). This approach allows analysis of the factorial portion before the axial portion is run. If curvature is insignificant based on the factorial portion, the additional runs are not necessary.

As shown in table 1, the number of coefficients in the quadratic model increases with k, and the number of trial batches required using a CCD begins to increase significantly for $k > 5$.

Table 1. Number of runs required for CCD experiment for k = 2 to 5 factors

k	Factorial	Axial	Center*	Total
2	4	4	5	13
3	8	6	5	19
4	16	8	5	29
5	16**	10	5	31

*assumes 3 CP for factorial portion and 2 CP for axial portion

**for k=5, a half-fraction of the full factorial is sufficient to estimate all linear terms and 2-factor interactions without confounding. Thus, 2^{5-1} or 16 factorial points are usually sufficient

Therefore, using a CCD to optimize a concrete mixture of more than six components may be uneconomical. In such cases, one could identify the most important factors and limit them to five or fewer. For example, if the cementitious materials and chemical admixtures were the most important components, they would be varied, while the amounts of coarse and fine aggregate would be held constant.

Laboratory experiments were conducted using the mixture and factorial approaches to see if one was more appropriate for concrete mixture optimization. The experiments are described in chapters 3 and 4. The adaptability of each method for use as an interactive, Web-based program was also considered in developing the COST software, described in chapter 5.

2.3 Model Fitting and Validation

The polynomial models described in sections 2.2.1 and 2.2.2 are fit to data using analysis of variance (ANOVA) and least squares techniques [9]. Many statistical software packages have the capability to perform these analyses and fits. Once a model has been fit, it is important to verify the adequacy of the chosen model quantitatively and graphically.

Although the models (polynomials) are slightly different for the classical mixture approach and the factorial approach, many of the steps involved in model selection and fitting are the same. The first step in each case is to perform ANOVA to select the appropriate type of model (linear, quadratic, etc.). Sequential F-tests are performed, starting with a linear model and adding terms (quadratic, and higher if appropriate). Under the "Source" column of the ANOVA table, the line labeled "Linear" indicates the significance of adding linear terms, and the line labeled "Quadratic" indicates the significance of adding quadratic terms. The column labeled "DF" shows the degrees of freedom for each source. The F-statistic is calculated for each type of model, and the highest order model with significant terms normally would be chosen. Significance is judged by determining if the probability that the F-statistic calculated from the data exceeds a theoretical value. The probability decreases as the value of the F-statistic increases. If this probability is less than 0.05 (typically, although other levels of significance could be used), the terms are significant and their inclusion improves the model. An example of an ANOVA table for sequential model sum of squares is shown in table 2.

Table 2. Example of ANOVA sequential model sum of squares

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	329.27	1	329.27	–	–
Linear	96.94	5	19.39	45.64	< 0.0001
Quadratic	6.36	15	0.42	1.00	0.5017
Special Cubic (aliased)	3.35	7	0.48	1.26	0.3727
Cubic (aliased)	0.00	0	–	–	–
Residual	3.03	8	0.38	–	–
Total	438.95	36	12.19	–	–

In this example, the linear model is the highest order model with significant terms (Prob > F is less than 0.05); therefore, it would be the recommended model for this data. Typically, the selected model will be the highest order polynomial where additional terms are significant and the model is not aliased.

Once the type of model (e.g., linear, quadratic, etc.) is selected, the second step is to perform a lack-of-fit test, also using ANOVA, to compare the residual error to the pure error from replication. Table 3 is an example of ANOVA for lack of fit. If residual error significantly exceeds pure error, the model will show significant lack of fit, and another model may be more appropriate.

The desired result in a lack-of-fit test is that the model selected in step 1 will not show significant lack of fit (i.e., the F test will be insignificant). If the "Prob > F" value is less than the desired significance level (often .05), this indicates significant lack of fit.

Several summary statistics can be calculated for a model and used to compare models or verify model adequacy. These statistics include root mean square error (RMSE), adjusted r^2,

Table 3. Example of ANOVA lack-of-fit test

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Linear	6271.93	22	285.09	1.17	0.4335
Quadratic	2164.86	7	309.27	1.27	0.3703
Special Cubic (aliased)	0.00	0	–	–	–
Cubic (aliased)	0.00	0	–	–	–
Pure Error	1950.91	8	243.86	–	–

predicted r^2, and prediction error sum of squares (PRESS). The RMSE is the square root of the mean square error, and is considered to be the standard deviation associated with experimental error. The adjusted r^2 is a measure of the amount of variation about the mean explained by the model, adjusted for the number of parameters in the model[2]. The predicted r^2 measures the amount of variation in new data explained by the model. PRESS measures how well the model fits each point in the design. To calculate PRESS, the model is used to estimate each point using all of the design points except the one being estimated. PRESS is the sum of the squared differences between the estimated values and the actual values over all the points. A good model will have a low RMSE, a large predicted r^2, and a low PRESS.

After a model is selected, standard linear regression techniques (least squares) are used to fit the model to the data. ANOVA is performed and an overall F-test and lack-of-fit test confirm the applicability of the model. Summary statistics (r^2, adjusted r^2, PRESS, etc.) and the standard error for each model coefficient also are calculated.

For the factorial approach, an iterative model fitting process was used in this research. First, a full quadratic (or linear, if applicable) model is assumed, and significance tests (t-tests) are performed on each model coefficient. Insignificant terms are removed and the fitting process is repeated using a partial quadratic (or linear, if applicable) model. The significance tests are repeated and insignificant terms, if any, are removed. The process is repeated until there are no insignificant terms. At this point, if the model contains two-factor interaction or quadratic terms, it is checked for hierarchy. Hierarchical terms are linear terms that may be insignificant by themselves but are part of significant higher order terms. For example, x_1 and x_3 are hierarchical terms of x_1x_3, a two-factor interaction term. If x_1x_3 is a significant term in the model, x_1 and x_3 are usually included in the model to maintain hierarchy. A hierarchical model allows for conversion of models between different sets of units (for a model involving temperature, conversion from F to C, for example).

Table 4 shows an ANOVA table for a selected model from a factorial experiment. Using the iterative approach, a reduced quadratic model was fit to the data. Note that terms B, C, and E are not significant ("Prob > F" >.05) but were added back into the model to make it hierarchical.

[2]The adjusted r^2 differs from the "standard" r^2, which is not adjusted for the number of parameters. The standard r^2 can be made larger by adding more parameters to the model. This does not necessarily mean the model with more parameters is a better model.

Table 4. Example of ANOVA model fitting for 1-day strength

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	240.87	8	30.11	27.76	< 0.0001
A	213.26	1	213.26	196.66	< 0.0001
B	0.48	1	0.48	0.45	0.5113
C	0.04	1	0.04	0.04	0.8433
E	2.06	1	2.06	1.90	0.1819
A^2	6.20	1	6.20	5.72	0.0257
AC	5.15	1	5.15	4.75	0.0404
AE	7.16	1	7.16	6.60	0.0175
BC	6.51	1	6.51	6.00	0.0227
Residual	23.86	22	1.08	–	–
Lack of fit	19.08	18	1.06	0.89	0.6248
Pure error	4.78	4	1.19	–	–
Corr. total	264.72	30			

Once the model fitting is performed, the next step is residual analysis to validate the assumptions used in the ANOVA. This analysis includes calculating case statistics to identify outliers and examining diagnostic plots such as normal probability plots and residual plots. If these analyses are satisfactory, the model is considered adequate, and response surface (contour) plots can be generated. Contour plots can be used for interpretation and optimization.

2.4 Optimization

When appropriate models have been established, several responses can be optimized simultaneously. Optimization may be performed using mathematical (numerical) or graphical (contour plot) approaches. Generally, graphical optimization is limited to cases in which there are only a few responses.

Numerical optimization requires defining an objective function (called a desirability or score function) that reflects the levels of each response in terms of minimum (zero) to maximum (one) desirability. One approach uses the geometric mean of the desirability functions for each individual response, where n is the number of responses to be optimized [10]:

$$D = (d_1 \times d_2 \times \ldots \times d_n)^{\frac{1}{n}} \tag{7}$$

Another approach is to use a weighted average of desirability functions:

$$D = \frac{(w_1 \times d_1 + w_2 \times d_2 + \ldots + w_n \times d_n)}{n} \tag{8}$$

where n is the number of responses and w_i are weighting functions ranging from 0 to 1.

Several types of desirability functions can be defined. Common types of desirability functions are shown in figure 5.

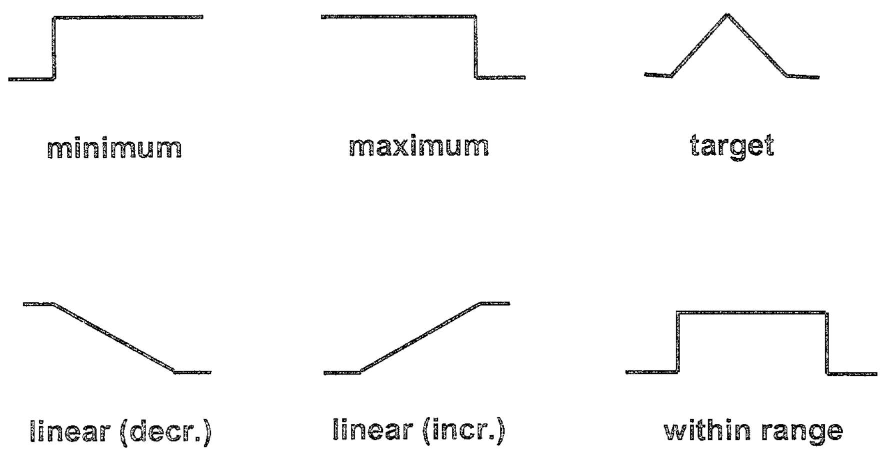


Figure 5. Examples of desirability functions

These functions can also be expressed mathematically as well. For example, a linear desirability function where minimum is best would be expressed as:

$$d_i = \left[\frac{B_i - Y_i}{B_i - A_i}\right]^{w_i} \tag{9}$$

for the range $A_i \leq Y_i \leq B_i$ and with $w_i = 1$.

Once the desirability functions (and weights, if used) are defined for each response, optimization may proceed.

As an alternative to rigorous numerical methods, desirability can be evaluated by superimposing a grid of points at equal spacing over the experimental region and evaluating desirability at each point. The point(s) of maximum desirability can be found by sorting the results or by creating contour plots of desirability over the grid area.

CHAPTER 3
Laboratory Experiment Using Mixture Approach

3.1 Introduction

This chapter describes the application of a statistically designed mixture experiment to the problem of optimizing properties of HPC. In a mixture experiment, the total amount (mass or volume) of the mixture is fixed, and the factors or component settings are proportions of the total amount. For concrete, the sum of the volume fractions is constrained to sum to one (as in the ACI mix design approach). Since the volume fractions must sum to unity, the component variables in a mixture experiment are not independent.

A mixture experiment was designed to find the optimum proportions for a concrete mix meeting the following conditions: slump of 50 to 100 mm, 1-day compressive strength of 22.06 MPa, 28-day compressive strength of 51.02 MPa, 42-day charge passed in American Society for Testing and Materials (ASTM) C1202 "rapid chloride" test (RCT) less than 700 coulombs, and minimum cost. The materials (components) used included water, cement, silica fume, high-range water-reducing admixture (HRWRA), coarse aggregate, and fine aggregate.

3.2 Selection of Materials, Proportions, and Constraints

The proportions for the six-component mixture experiment initially were selected in terms of volume fraction and converted to weights for batching. The minimum and maximum levels of each component were chosen based on typical volume fractions for non-air-entrained concrete with the constraint that the volume fractions sum to unity. In addition to the individual constraints on each component, the paste fraction of the concrete (water, cement, silica fume, and HRWRA) was required to range from 25 to 35 percent by volume. Although air is incorporated into concrete during mixing, it is not an initial component and therefore was not considered to be a component of the mixture. Ignoring the air content as a mix component affects yield calculations, but these are not important for the small trial batches and can be adjusted later after a final mix is selected.

The materials used in this study included a Type I/II portland cement, tap water, #57 crushed limestone coarse aggregate, natural sand, silica fume (in slurry form), and a naphthalene sulfonate-based HRWRA meeting ASTM C494 Type F/G. The final volume fraction ranges of the 6 mixture components are shown in table 5. The volume fractions were converted to corresponding weights using the specific gravities and percent solids (where applicable) obtained from laboratory testing or from the material supplier.

3.3 Experiment Design Details

Selecting an appropriate experiment design depends on several criteria, such as ability to estimate the underlying model, ability to provide an estimate of repeatability, and ability to check the adequacy of the fitted model. The "best" experiment design depends on the choice of an

Table 5. Material volume fraction ranges for mixture experiment

Component	ID	Minimum volume fraction	Maximum volume fraction
Water	x_1	.16	.185
Cement	x_2	.13	.15
Silica fume	x_3	.013	.027
HRWRA	x_4	.0046	.0074
Coarse aggregate	x_5	.40	.4424
Fine aggregate	x_6	.25	.2924

underlying model which will adequately explain the data. For this experiment, the following quadratic Scheffé polynomial was chosen as a reasonable model for each property as a function of the six components:

$$y = b_1 x_1 + \ldots + b_6 x_6 + b_{12} x_1 x_2 + \ldots + b_{56} x_5 x_6 + e \tag{10}$$

This model is an extension of equation 4 for the 6-component case. Because there are 21 coefficients in the model, the design must have at least 21 runs (21 distinct mixes) to estimate these coefficients. In addition to the 21 required runs, 7 additional runs (distinct mixes) were included to check the adequacy of the fitted model, and 5 mixes were replicated to provide an estimate of repeatability. The replicates were required to test the statistical significance of the fitted coefficients. Finally, a single mix was replicated during each week of the experiment to check statistical control of the fabrication and measurement process. In all, a total of 36 mixes were planned.

Commercially available computer software for experiment design was used to design and analyze the experiment. The program selected 36 points from a list of candidate points that is known to include the best points for fitting a quadratic polynomial. A modified-distance design was chosen to ensure that the design selected could estimate the quadratic mixture model while spreading points as far away as possible from one another.

Table 6 summarizes the mixture proportions used in the experiment. The run order was randomized to reduce the effects of extraneous variables not explicitly included in the experiment. The first three mixes were repeated at the end of the program (runs 37, 38, and 39), because an incorrect amount of water was used in batching the mixes. The test results from the incorrectly batched mixes were not included in the subsequent analysis. Of the final 36 mixes, 8 were replicates (one each from mixes 5, 11, 20, 38, 71 and three from mix 127).

3.4 Specimen Fabrication and Testing

Thirty-nine batches of concrete, each approximately .04 m^3 in volume, were prepared over a four-week period. A rotating-drum mixer with a 0.17 m^3 capacity was used to mix the concrete.

Table 6. Mixture proportions for mixture experiment

Design ID	Run Order	Water (kg)	Cement (kg)	Silica Fume (kg)	HRWRA (l)	Coarse Aggregate (kg)	Fine Aggregate (kg)	w/(c+sf)
5(r)	7, 22	122.3	312.9	45.4	3.52	867.6	506.3	0.35
11(r)	6, 23	141.4	312.9	21.9	3.52	845.3	506.3	0.43
13	15	122.3	312.9	21.9	3.52	810.1	592.2	0.37
15	2*, 38	126.6	361.1	45.4	5.66	810.1	506.3	0.32
16	8	122.3	312.9	21.9	3.52	895.9	506.3	0.37
20(r)	13, 34	141.4	312.9	21.9	3.52	810.1	541.8	0.43
22	4	141.4	354.8	21.9	3.52	810.1	506.3	0.38
28	16	122.3	312.9	45.4	3.52	810.1	563.8	0.35
37	30	122.3	337.0	45.4	5.66	810.1	537.9	0.33
38(r)	3*, 26, 39	135.0	341.1	45.4	3.52	810.1	506.3	0.36
48	28	131.8	312.9	21.9	5.66	810.1	561.2	0.41
63	27	131.8	312.9	45.4	5.66	836.6	506.3	0.38
65	31	122.3	337.0	45.4	5.66	841.7	506.3	0.33
66	25	122.3	312.9	45.4	5.66	836.0	532.2	0.35
70	29	122.3	361.1	21.9	4.59	810.1	548.8	0.33
71(r)	5, 35	122.3	361.1	21.9	5.66	829.9	526.1	0.33
78	11	141.4	312.9	45.4	5.66	810.7	506.9	0.41
87	24	122.3	312.9	21.9	3.52	853.0	549.2	0.37
89	19	122.3	337.0	21.9	3.52	810.1	571.9	0.35
91	9	141.4	312.9	21.9	5.66	824.9	521.1	0.43
98	17	122.3	337.0	21.9	3.52	875.7	506.3	0.35
101	10	130.8	361.1	21.9	3.52	832.8	506.3	0.35
103	14	122.3	361.1	21.9	4.59	852.6	506.3	0.33
110	21	130.8	361.1	21.9	3.52	810.1	529.0	0.35
116	33	131.8	312.9	45.4	5.66	810.1	532.8	0.38
123	36	122.3	337.0	33.6	4.59	834.4	530.6	0.34
127(c)	1*, 12, 18, 32, 37	131.5	335.8	21.9	4.59	829.9	526.1	0.38
163	20	126.6	323.3	27.8	5.12	857.5	513.6	0.37

Notes: Aggregate masses are in dry condition
(r) replicated mix
(c) control mix
* mix that was repeated due to incorrect batching

Each batch included sufficient concrete for two slump tests, two fresh air content (ASTM C231) tests, two unit weight tests, and ten 100 mm x 200 mm cylinders. The cylinders were fabricated in accordance with ASTM C192. To obtain adequate consolidation, cylinders for concretes with slumps less than 50 mm were vibrated on a vibrating table; otherwise, the cylinders were rodded. The cylinders were covered with plastic and left in the molds for 22 hours, after which they were stripped and placed in limewater-filled curing tanks for moist curing at 23 ±2°C.

Compressive strength tests (ASTM C39) were conducted on the cylinders at the ages of 1 day and 28 days. In most cases, three cylinders were tested for each age. A fourth test was performed in some cases if one result was significantly lower or higher than the others. Before testing, the cylinder ends were ground parallel to meet the ASTM C39 requirements using an end-grinding machine designed for this purpose. The three remaining cylinders from each batch were used for "rapid chloride" testing according to ASTM C1202. Three 50-mm thick slices taken from the middle sections of the concrete cylinders were tested at an age of 42 days.

3.5 Results and Analysis

3.5.1 Measured Responses

The average values for slump, 1-day strength, 28-day strength, and RCT charge passed for each batch are shown in table 7, along with the estimated cost per cubic meter of concrete. The cost of each batch was calculated from the mix proportions using approximate costs for each component material obtained from a local ready-mix concrete producer. For each of the four responses, a model was fit using least-squares methods, validated (by examining the residuals for trends and outliers), and interpreted graphically using contour and trace plots. The statistical analysis is described in detail for 28-day strength. The analyses for the other properties were performed in a similar manner. ANOVA tables, model statistics, and plots for all responses are included in Appendix A.

3.5.2 Model Identification and Validation for 28-Day Strength

In this section, a detailed description of the process of model identification and validation is provided for the response 28-day strength. The models for other responses were identified and validated in the same way. Those models are presented in the next section.

The first step in the analysis is to select a plausible model. Even though the experiment design used permits estimation of a quadratic model, a linear model may provide a better fit to the data. ANOVA is used to assess the different models.

ANOVA results for 28-day strength are shown in table 8. In this table, each row tests whether the coefficients of certain model terms are equal to zero. For example, the row with source "Linear" tests whether the coefficients of the linear terms are equal to zero. A low value (say, less than 0.05) of "Prob > F", also called the p-value, supports the conclusion that the coefficients differ from zero and should be included in the model. For the data in table 7, the "Prob > F" is 0.0011; therefore, the linear terms should be included in the model. The row with

Table 7. Test results and costs (mixture experiment)

Design ID	Run	Slump (mm)	1-Day Str (MPa)	28-Day Str (MPa)	42-Day RCT (coulombs)	Cost ($/ m^3)
22	4	67	21.5	48.2	1278	95.18
71	5	57	27.0	55.2	862	102.22
11	6	102	16.8	48.5	1162	91.32
5	7	13	22.4	48.5	387	118.85
16	8	35	21.6	53.1	776	92.20
91	9	200	16.8	60.4	1027	96.89
101	10	22	26.6	53.6	744	96.24
78	11	127	19.2	51.7	492	123.56
127	12	99	21.5	50.2	842	96.67
20	13	118	18.2	50.9	903	91.32
103	14	64	27.4	54.6	583	99.42
13	15	57	21.8	53.2	684	92.20
28	16	29	22.2	53.6	292	118.85
98	17	32	25.3	51.9	604	94.41
127	18	92	22.3	54.1	847	96.67
89	19	38	21.8	54.3	720	94.41
163	20	95	22.1	60.8	554	103.80
110	21	51	24.7	53.2	792	96.24
5	22	25	23.4	54.1	348	118.85
11	23	114	16.5	48.0	968	91.32
87	24	67	22.9	51.0	700	92.20
66	25	76	24.7	59.8	316	124.44
38	26	29	23.0	53.2	390	120.85
63	27	124	21.7	55.2	302	123.99
48	28	171	23.0	58.1	682	97.34
70	29	51	27.5	54.5	505	99.42
37	30	35	27.3	56.0	245	126.65
65	31	32	27.2	51.1	310	126.65
127	32	121	22.4	57.2	636	96.67
116	33	114	23.9	56.2	356	123.99
20	34	127	18.6	51.6	820	91.32
71	35	108	28.8	65.3	553	102.22
123	36	99	26.6	61.0	340	110.53
127	37	102	24.2	54.6	640	96.67
15	38	51	28.8	58.1	239	128.68
38	39	25	23.6	54.5	332	120.85

Table 8. Sequential model sum of squares for 28-day strength (mixture experiment)

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	106212.98	1	106212.98	–	–
Linear	257.52	5	51.50	5.46	0.0011
Quadratic	135.19	15	9.01	0.92	0.5665
Residual	147.62	15	9.84	–	–
Total	106753.31	36	2965.37	–	–

source "Quadratic" tests whether any quadratic coefficients differ from zero. Since the "Prob >F" of 0.5667 exceeds 0.05, the quadratic terms should not be included in the model.

A lack-of-fit test can also be performed using ANOVA. To do so, the residual sum of squares is partitioned into lack-of-fit and pure error (from replicates) components. The mean squares and F statistic are calculated, and the "Prob > F" is determined. The desired result is an insignificant lack-of-fit, indicated by a "Prob > F" greater than 0.05. For 28-day strength, the lack-of-fit test for the linear model gives "Prob > F" equal to 0.7193, which is insignificant (the ANOVA tables for the lack-of-fit test for 28-day strength and the other responses are provided in Appendix A).

The resulting linear model for 28-day strength (y_1), fit by least squares, is

$$\hat{y}_1 = -45.22x_1 + 89.15x_2 - 3.81x_3 + 1972x_4 + 38.36x_5 + 87.19x_6 \tag{11}$$

with the residual standard deviation $s = 3.07$ MPa. The residual standard deviation s is defined as:

$$s = \sqrt{\frac{\sum (y_i - \hat{y}_i)^2}{n-p}} \tag{12}$$

where the number of observations $n = 36$ and the number of parameters in the fitted model $p = 6$. A value of s near the repeatability value (replicate standard deviation) is an indication of an adequately fitting model. The repeatability value is 3.39 MPa, which is close to s.

Residual plots are used to validate the fitted model. The residuals are the deviations of the observed data from the fitted values, $y_i - \hat{y}_i$. The residual $y_i - \hat{y}_i$. estimates the error terms e_i in the model. The e_i are assumed to be random and normally distributed with mean zero and constant standard deviation. The residuals, which estimate these errors, should exhibit similar properties. Essentially, an adequate model should capture all information in the data leaving structureless, random residuals. If structure remains in the residuals, residual plots often will suggest how to modify the model to remove the structure. In this study, plots of residuals versus run sequence and a plot of the control mix results revealed a linear trend in the data for each response. However, because the run sequence was randomized, this trend had little impact on the fitted models.

3.5.3 Models for Other Responses

Using the same procedure described above for 28-day strength, the following models were fit to slump (y_2), 1-day strength (y_3), and 42-day charge passed (y_4):

$$\hat{y}_2 = 2166.5x_1 - 2390.5x_2 - 3401.2x_3 + 24268x_4 - 204.83x_5 + 169.90x_6 \quad \textbf{(13)}$$

$$\begin{aligned}\hat{y}_3 = &-1209.1x_1 + 1775.9x_2 - 74.712x_3 - 11969x_4 + 59.589x_5 - 105.24x_6 \\ &+ 4214.9x_1x_6 - 5603.1x_2x_6 + 43782x_3x_4 + 44781x_4x_6\end{aligned} \quad \textbf{(14)}$$

$$\ln(\hat{y}_4) = 20.82x_1 + 0.629x_2 - 52.33x_3 - 23.40x_4 + 7.24x_5 + 3.19x_6 \quad \textbf{(15)}$$

Linear models were adequate for all responses except 1-day strength, for which the fitted model includes 4 quadratic terms that were found to be significant. A natural logarithm transform was used to model 42-day charge passed because residual plots showed that the standard deviation of the data for charge passed was proportional to the mean.

3.6 Optimization

3.6.1 Graphical Interpretation

Once a valid model is identified, it can be interpreted graphically using response trace plots and contour plots. A response trace plot is shown in figure 6. This figure consists of six overlaid plots, one for each component. For a given component, the fitted value of the response is plotted as the component is varied from its low to high setting in the constrained region, while the other components are held in the same relative ratio as a specified reference mixture, here the centroid. The plot shows the "effect" of changing each component on 28-day strength. As expected, increasing the amount of water decreased strength, while increasing the amount of cement increased strength. HRWRA had the largest effect with higher amounts of HRWRA yielding higher strength. This may be due to the improved dispersion of the cement and silica fume caused by higher amounts of HRWRA. Surprisingly, an increase in silica fume appears to reduce strength. However, this apparent reduction may not be significant when compared to the underlying experimental error.

Contour plots are used to identify conditions that give maximum (or minimum) response. Because contour plots can only show three components at a time (the others components are set at fixed conditions), several must be examined. Figure 7 is a contour plot of 28-day strength for water, cement, and HRWRA, with the other components fixed at their centroid values. The plot indicates that strength increases rapidly by increasing HRWRA, confirming the result from the

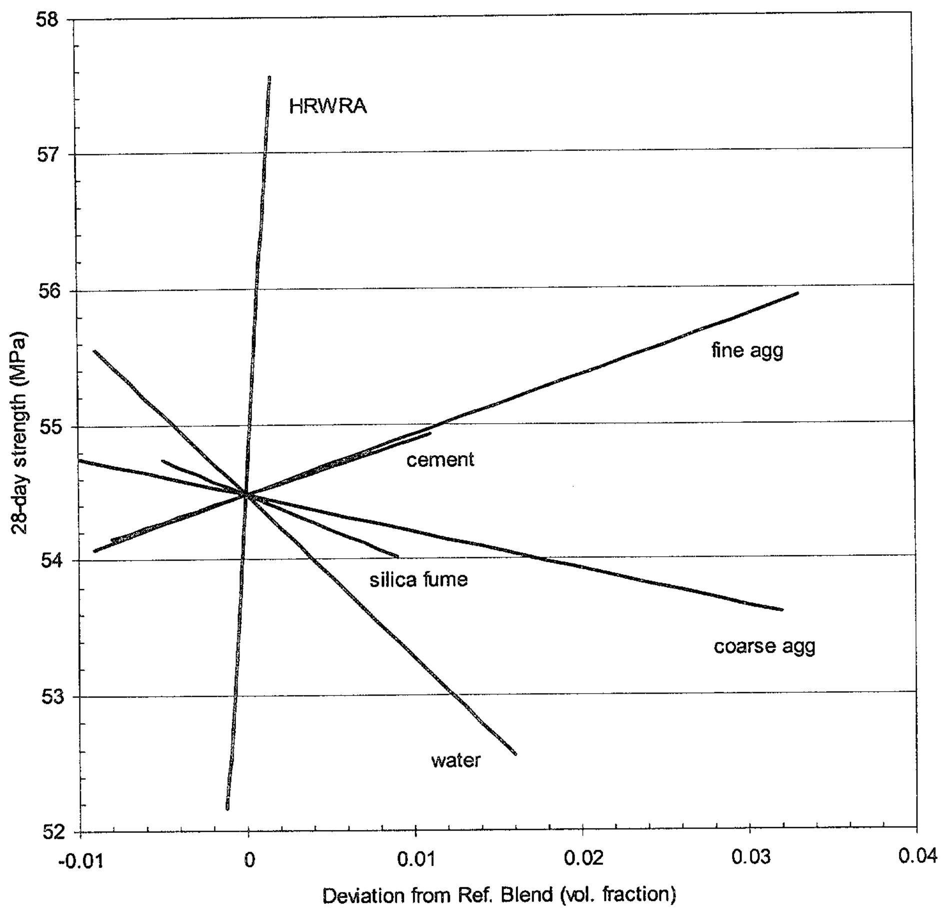


Figure 6. Response trace plot for 28-day strength (mixture experiment)

response trace plot. Therefore, in subsequent contour plots, HRWRA will be set at its high value.

Figure 8 shows a contour plot of 28-day strength in water, cement, and silica fume, and figure 9 shows a contour plot in water, coarse aggregate, and fine aggregate. In each case, HRWRA is fixed at its high value, and the other components are fixed at the centroid settings. These plots show that strength increases for low water, high cement, low silica fume, low coarse aggregate, and high fine aggregate.

The best overall settings for 28-day strength can be found using the contour plot in figure 10, which shows 28-day strength in silica fume, coarse aggregate, and fine aggregate at the best settings of water, cement, and HRWRA. The best settings (expressed as volume fractions) are water = 0.160, cement = 0.150, silica fume = 0.013, HRWRA = 0.0074, coarse aggregate = 0.400, and fine aggregate = 0.270, with a predicted strength of 59.53 MPa.

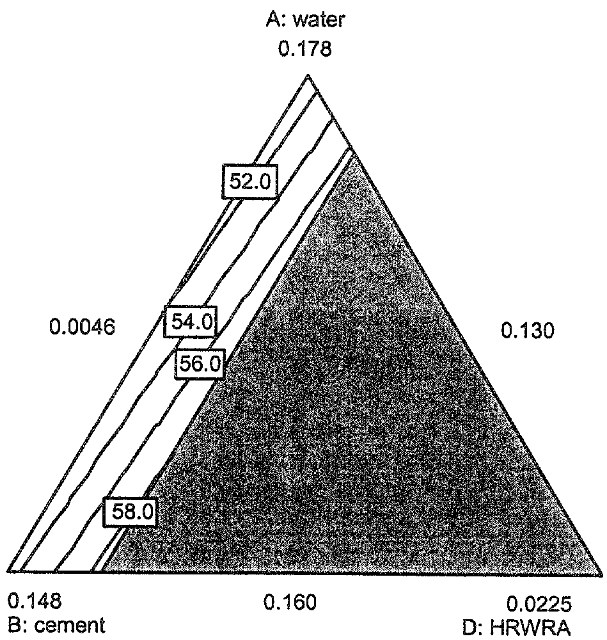


Figure 7. Contour plot for 28-day strength in water, cement, and HRWRA

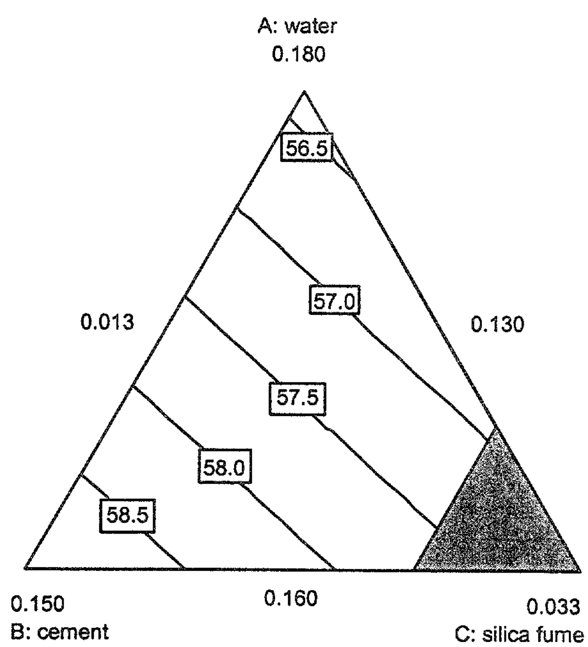


Figure 8. Contour plot for 28-day strength in water, cement, and silica fume

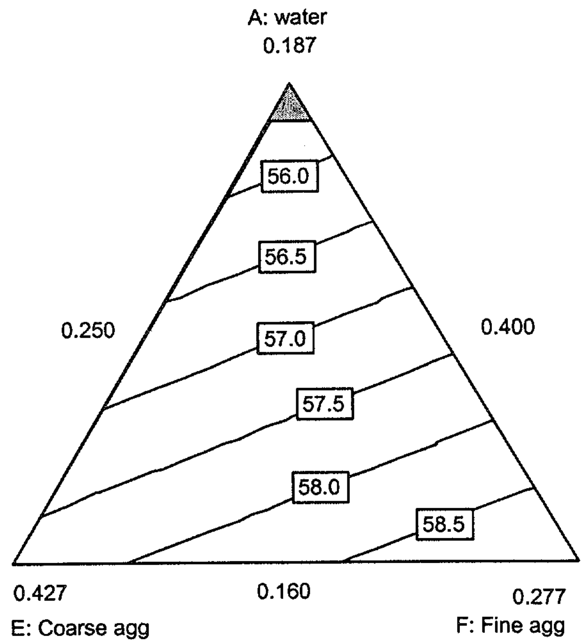


Figure 9. Contour plot for 28-day strength in water, coarse aggregate, and fine aggregate

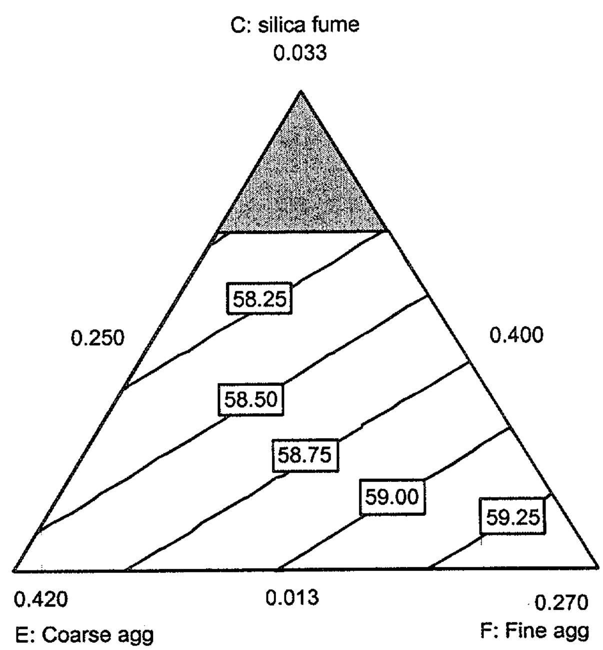


Figure 10. Contour plot for 28-day strength in silica fume, coarse aggregate, and fine aggregate

3.6.2 Numerical Optimization

The optimum concrete mix is defined here as that mix which minimizes cost while meeting specified performance criteria. Numerical optimization using desirability functions [10] can be used to find the optimum mixture proportions in this situation. A desirability function must be defined for each response (property). The desirability function takes on values between 0 and 1, and may be defined in several ways. Figure 11 shows the desirability functions defined for the responses in this experiment. Minimum and maximum specifications are used for strength and RCT, resulting in desirability functions with values of 1 above the minimum or below the maximum, and 0 otherwise. For example, for 1-day strength the desirability value is 0 below 22.06 MPa and 1 above 22.06 MPa. At 34.48 MPa, well beyond the maximum value observed in the data, the desirability becomes 0. Desirabilities for 28-day strength and 42-day RCT are defined similarly. For slump, a range of 50 to 100 mm was specified, but the midpoint of this range, 75 mm was selected as the most desirable value (the target value). Therefore, a desirability of 1 is given to the target value of 75 mm, with a linear decrease in desirability to a value of zero at the lower and upper specification limits (see figure 11). Since cost is to be minimized, the desirability function for cost decreases linearly over the range of costs observed in the data, as shown in figure 11.

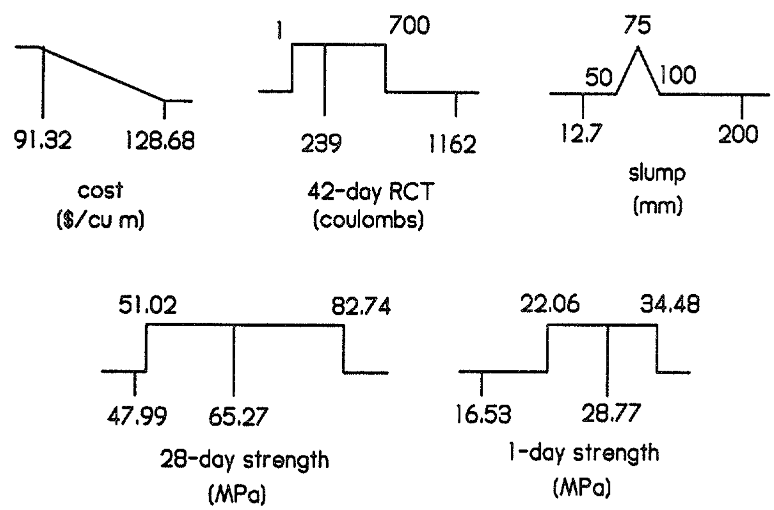


Figure 11. Desirability functions for responses in mixture experiment

The individual desirabilities can be expressed mathematically in terms of the predicted response values (see equation 9, page 14), which can be calculated for each mixture in the experiment. In this study, the overall desirability D was defined as the geometric mean of the individual desirability functions d_i over the feasible region of mixtures [10]:

$$D = (d_1 d_2 d_3 d_4 d_5)^{1/5} \tag{16}$$

The optimal mix is the one with a maximum value of D, which may be determined in several ways. The simplest (but crudest) approach is to select the mixture with the largest value of D from the design points in the experiment. Another approach is to consider D as a response and fit a model to it (as one would fit a model to 28-day strength). A third approach is to use numerical search algorithms to find the maximum value of D [12]. The third approach was used here.

Based on the experimental results, the mix which maximizes D, expressed in volume fractions, is water = 0.160, cement = 0.130, silica fume = 0.013, HRWRA = 0.0049, coarse aggregate = 0.401, and fine aggregate = 0.290, at a cost of \$93.01 per m^3. The overall desirability value for this mix is 0.964, and the predicted response values are slump = 75 mm, 1-day strength = 22.07 MPa, 28-day strength = 54.72 MPa, and 42-day RCT value = 631 coulombs.

3.6.3 Accounting for Uncertainty

If the fitted functions for each property were known without error, the analysis would be complete. However, there is uncertainty in the fitted functions, because they are estimated from a sample of data. For example, at the current mix the predicted 1-day target strength is 22.07 ±1.01 MPa. The uncertainty provided is for a 95 percent confidence interval, i.e., we are 95 percent confident that the interval (21.06, 23.08) contains the true 1-day target strength for this mix. If this mix is used, it is quite possible that actual 1-day strength results would fall below the minimum acceptable value of 22.06 MPa. Therefore, each specification must be modified to account for uncertainties in the fitted functions. The uncertainties in the properties of the current best mix can be used to modify the constraints (performance criteria) and identify a revised optimal mix based on these new constraints. The revised mix must then be checked to see that the original specifications are met.

The predicted values and 95 percent uncertainties for the remaining responses at the current best mix are slump = 75 ±17 mm, 28-day strength = 54.72 ±3.25 MPa, and ln(42-day RCT) = 6.448 ±0.162[1]. The modified constraints on the responses which take into account the uncertainties are 67 mm < slump < 83 mm, 1-day target strength > 23.07 MPa, 28-day target strength > 54.27 MPa, and ln(42-day RCT) < 6.389 (42-day RCT < 595 coulombs)[2]. Repeating the numerical optimization, the best mix for this new set of constraints (expressed as volume fractions) is water = 0.160, cement = 0.133, silica fume = 0.014, HRWRA = 0.0054, coarse aggregate = 0.409, and fine aggregate = 0.2786 at a cost of \$96.35. The predicted values and 95 percent uncertainties for this mix are slump = 76 ±15 mm, 1-day strength = 23.05 ±0.69 MPa, 28-day strength = 55.20 ±2.31 MPa, and ln(42-day RCT) = 6.404 ±0.114 (corresponding to a range of 539 to 678 coulombs). For this mix, the 95 percent confidence intervals for all responses meet the original specifications. Accounting for uncertainty increased the cost of the optimal mix by about 3 percent (\$93.01 to \$96.35). The value of optimization can be seen by comparing the cost of the optimal mix (\$96.35) with the range of costs for all mixtures in the experiment (\$91.32 to \$128.68 per m^3).

---

[1]The predicted value and uncertainty for ln(42-day RCT) are provided because the ln transform was used in the model for RCT. The actual 95% confidence interval for 42-day RCT ranges from 537 to 742 coulombs with a predicted value of 631 coulombs.

[2]The modified constraints are calculated by adding the uncertainty to the original lower bound constraint, or subtracting the uncertainty from the original upper bound. Thus, for slump, the new lower bound is 50 + 17 = 67 mm, and the new upper bound is 100 − 17 = 83 mm. For 1-day strength, which only has a lower bound, the new constraint is 22.06 + 1.01 = 23.07 MPa.

CHAPTER 4
Laboratory Experiment Using Factorial Approach

4.1 Introduction

This chapter describes the application of factorial experiment design to the problem of concrete mixture optimization. In a mixture, the total amount (mass or volume) of the product is fixed, and the settings of each of the q components are proportions. Because the total amount is constrained to sum to one, the component variables are not independent. However, the q components can be reduced to $q-1$ mathematically independent variables using the ratio of two components as an independent variable [8]. In the case of concrete, w/c is a natural choice for this ratio variable. If this strategy is adopted, a factorial approach may be applied.

4.2 Selection of Materials, Proportions, and Constraints

The materials used in this experiment were identical to those used in the mixture experiment (chapter 3): Type I cement, tap water, #57 crushed limestone, natural sand, silica fume (slurry), and naphthalene-sulfonate-based HRWRA. The six components were reduced to five independent variables: x_1 = w/c (by mass), x_2 = fine aggregate volume fraction, x_3 = coarse aggregate volume fraction, x_4 = HRWRA volume fraction, x_5 = silica fume volume fraction.

The volume fraction ranges for coarse aggregate, fine aggregate, HRWRA, and silica fume were the same as used in the mixture experiment. The range of w/c (by volume) was calculated from the volume fraction limits of the mixture experiment. The lower limit of w/c was $0.16 \div 0.15 = 1.067$, and the upper limit was $0.185 \div 0.13 = 1.423$. These limits were equated to coded limits of -1.5 to $+1.5$ to give the most similar experimental region to that of the mixture experiment. Table 9 shows the settings of each variable corresponding to coded values of -1 and $+1$.

Table 9. Variable settings corresponding to coded values (factorial experiment)

Variable	ID	Low Setting (coded value = -1)	High Setting (coded value = 1)
w/c ratio	x_1	1.1263 (≅ 0.36 by mass)	1.3637 (≅ 0.43 by mass)
Fine aggregate	x_2	0.2571	0.2853
Coarse aggregate	x_3	0.4071	0.4353
HRWRA	x_4	0.0051	0.0069
Silica fume	x_5	0.0153	0.0247

For the aggregates, HRWRA, and silica fume, volume fractions were converted to batch masses (batch volume for HRWRA) based on total batch size and material properties. The batch masses of water and cement were calculated by constraining the sum of volume fractions of all six components to sum to one. This gives two equations in two unknowns (the other equation being the w/c expressed volumetrically) that can be solved for volume fraction of water and volume fraction of cement. Entrapped air was ignored in these calculations, although in practice it will affect yield calculations and an overall adjustment to the mixture proportions may be necessary for proper yield.

The performance criteria for the mix were as follows: slump between 50 and 100 mm, 1-day strength greater than 22 MPa, 28-day strength greater than 51 MPa, and charge passed in the RCT less than 700 coulombs. These are the same performance criteria used for the mixture experiment, except that the 1-day and 28-day strengths were rounded to 22 and 51 MPa (from 22.06 and 51.02 MPa used in the mixture experiment)[1].

4.3 Experiment Design Details

A central composite design (see chapter 2) was chosen for this experiment. The actual values for each variable (expressed in terms of volume fraction) corresponding to the coded levels ±1 are shown in table 10. A commercially available software package for experiment design and analysis was used to plan the experiment. Thirty-one batches were planned in two nearly orthogonal blocks. The first block consisted of a half-fraction of 16 factorial points[2] and 3 center points, and the second block consisted of 10 axial points and 2 center points. A total of five center points was chosen to allow use of the center point mixes as statistical control mixes to assess week-to-week variation, if any, over the five weeks of mixing (in addition to the use of center points as replicates to estimate pure error). The run order within each block was randomized to reduce the effect of uncontrolled variables. Center point runs were placed first and last (based on the total number of runs) with the remainder equally spaced, resulting in three center points in the factorial block and two center points in the axial block. The mixture proportions for each batch are shown in table 10.

One batch (run 3) was repeated at the end of the experiment because of suspiciously low strength values. A center point batch was included with the repeat to check statistical control. The results of the repeated batch were used in subsequent analyses.

4.4 Specimen Fabrication and Testing

The materials used in this study included a portland cement conforming to ASTM specification C150-94 Type I/II, a #57 crushed limestone coarse aggregate meeting grading requirements of AASHTO M43, a natural sand fine aggregate, silica fume (in slurry form), a naphthalene-sulfonate based HRWRA (ASTM C494-98 Type F/G), and municipal tap water. Thirty-one batches of concrete, each approximately 0.04 m^3 in volume, were prepared over a 6-week period. Each batch was prepared in accordance with mixing procedures set forth in ASTM C192-95.

---

[1]The mixture experiment was originally performed using English units with 1-day strength requirement of 3200 psi and 28-day strength requirement of 7400 psi.

[2]The 16 factorial points represent a half-fraction of the full factorial for 5 variables, which has $2^5 = 32$ points. The 2^{5-1} half-fraction can be used in this case because it is a Resolution V design that allows estimation of all linear coefficients and two-factor interactions without confounding.

Table 10. Mixture proportions (per m^3) for factorial experiment

Batch (run)	w/c	Fine Agg (kg)	Coarse Agg (kg)	HRWRA (L)	Silica Fume (kg)	Cement (kg)	Water (kg)
1	0.36	755.7	1098.7	6.90	54.3	408.7	146.1
2	0.36	755.7	1174.8	5.10	54.3	369.6	132.2
3	0.40	718.4	1136.8	6.00	44.0	394.9	156.1
4	0.40	718.4	1136.8	6.00	44.0	394.9	156.1
5	0.43	681.0	1098.7	6.90	54.3	405.2	175.4
6	0.43	755.7	1098.7	5.10	54.3	370.1	160.2
7	0.43	755.7	1098.7	6.90	33.6	380.2	164.6
8	0.43	681.0	1098.7	5.10	33.6	420.1	181.9
9	0.36	681.0	1098.7	5.10	54.3	453.1	162.0
10	0.40	718.4	1136.8	6.00	44.0	394.9	156.1
11	0.43	755.7	1174.8	5.10	33.6	345.0	149.4
12	0.36	681.0	1098.7	6.90	33.6	464.4	166.0
13	0.43	681.0	1174.8	5.10	54.3	370.1	160.2
14	0.36	755.7	1098.7	5.10	33.6	425.3	152.1
15	0.43	681.0	1174.8	6.90	33.6	380.2	164.6
16	0.36	755.7	1174.8	6.90	33.6	380.9	136.2
17	0.36	681.0	1174.8	6.90	54.3	408.7	146.1
18	0.36	681.0	1174.8	5.10	33.6	425.3	152.1
19	0.43	755.7	1174.8	6.90	54.3	330.1	142.9
20	0.40	718.4	1212.9	6.00	44.0	355.4	140.5
21	0.47	718.4	1136.8	6.00	44.0	357.2	168.1
22	0.40	793.1	1136.8	6.00	44.0	355.4	140.5
23	0.40	718.4	1136.8	7.80	44.0	392.4	155.1
24	0.40	718.4	1136.8	6.00	44.0	394.9	156.1
25	0.32	718.4	1136.8	6.00	44.0	441.7	141.3
26	0.40	718.4	1136.8	4.20	44.0	397.5	157.1
27	0.40	718.4	1136.8	6.00	23.3	408.1	161.3
28	0.40	718.4	1060.6	6.00	44.0	434.5	171.7
29	0.40	718.4	1136.8	6.00	44.0	394.9	156.1
30	0.40	718.4	1136.8	6.00	64.7	381.8	150.9
31	0.40	643.7	1136.8	6.00	44.0	434.5	171.7

Precautions were taken to compensate for mortar retained by the mixer, by "buttering" the mixer prior to preparing each batch. The concrete was mixed using a rotating-drum machine mixer with a 0.17 m^3 mixing capacity.

Each batch included sufficient concrete for 2 slump tests, 1 unit weight and air content test (ASTM C138 and ASTM C231), and 10 100 mm x 200 mm cylinders. All cylinders were fabricated in accordance with ASTM C192, except that external vibration (a vibrating table) was utilized for consolidation in lieu of rodding when slump was less than 50 mm. Immediately following casting, the cylinders were covered with plastic and left in the molds at room temperature for 24 ± 8 hours, after which they were removed from the molds and moist cured at 23 ± 2 °C until testing. Specimens were tested for compressive strength in accordance with ASTM C39 at the ages of 1 and 28 days. In most cases, three cylinders were tested at each age, however, where anomalies in either specimen condition or test results were evident, a fourth or fifth specimen may have been tested. Prior to compression testing, the ends of each cylinder were ground plane and parallel in accordance with ASTM C39 tolerances. Three of the remaining cylinders from each batch were used for the RCT testing. Testing was performed according to ASTM C1202, except that the 50 mm test specimens were cut from the middle of each cylinder instead of from the top. All RCTs were performed at an age of 42 days from casting.

4.5 Results and Analysis

4.5.1 Responses

The average values for slump, 1-day strength, 28-day strength, and charge passed (RCT) for each batch are shown in table 11, along with the estimated cost (dollars per cubic meter) of the concrete mixture. The costs were calculated from the mixture proportions for each batch, based on approximate component costs obtained from a local (mid-Atlantic) ready-mix concrete producer. Each response was analyzed individually by examining summary plots of the data (scatterplots and means plots), fitting a model using ANOVA and least-squares methods, validating the model by examining the residuals for trends and outliers, and interpreting the model graphically. A detailed discussion of the analysis procedure for 1-day strength is presented in the following 2 sections. The analyses for the other responses were performed in a similar manner. The models for the other responses are reported in section 4.5.4.

4.5.2 Exploratory Data Analysis for 1-Day Strength

One advantage of the factorial approach is the ability to perform an initial assessment of the data using graphical techniques such as raw data plots, means plots, scatterplots, and cube plots. These techniques are illustrated in figures 12-15 (for complete sets of plots for each response, see appendix B). A raw data plot of 1-day strength is shown in figure 12. This plot illustrates the variation in the response (1-day strength) over time, for each run. The control batch results,

Table 11. Test results and costs (factorial experiment)

Batch (run)	Slump (mm)	1-Day (MPa)	28-Day (MPa)	RCT (coul)	Cost ($/m3)
1	73	16.3	58.5	286	119.77
2	44	22.6	59.8	209	113.93
3	13	20.8	52.6	160	107.71
4	102	16.5	60.4	296	107.71
5	57	16.4	55.0	257	118.49
6	143	13.6	58.6	541	112.96
7	67	12.9	50.4	502	99.21
8	13	20.3	52.4	234	97.83
9	86	18.4	63.0	305	118.75
10	102	15.2	54.8	445	107.71
11	140	20.7	62.3	412	93.70
12	32	17.1	56.2	252	105.09
13	13	24.2	54.2	341	112.98
14	76	17.2	50.3	534	99.24
15	13	21.3	59.2	278	99.23
16	13	20.9	60.5	206	100.27
17	57	18.8	56.6	315	119.78
18	29	21.9	58.3	355	99.26
19	35	16.1	62.9	230	114.36
20	38	19.0	58.6	211	105.49
21	117	14.5	53.9	458	104.63
22	67	17.8	62.4	294	105.48
23	64	19.9	67.5	268	111.16
24	16	26.4	58.5	189	107.71
25	79	19.0	57.0	257	111.52
26	64	19.1	50.9	273	104.27
27	152	16.8	54.4	705	90.56
28	95	20.2	53.3	307	109.93
29	35	18.4	55.2	162	107.71
30	102	17.4	50.4	332	124.87
31	76	18.4	55.2	277	109.95

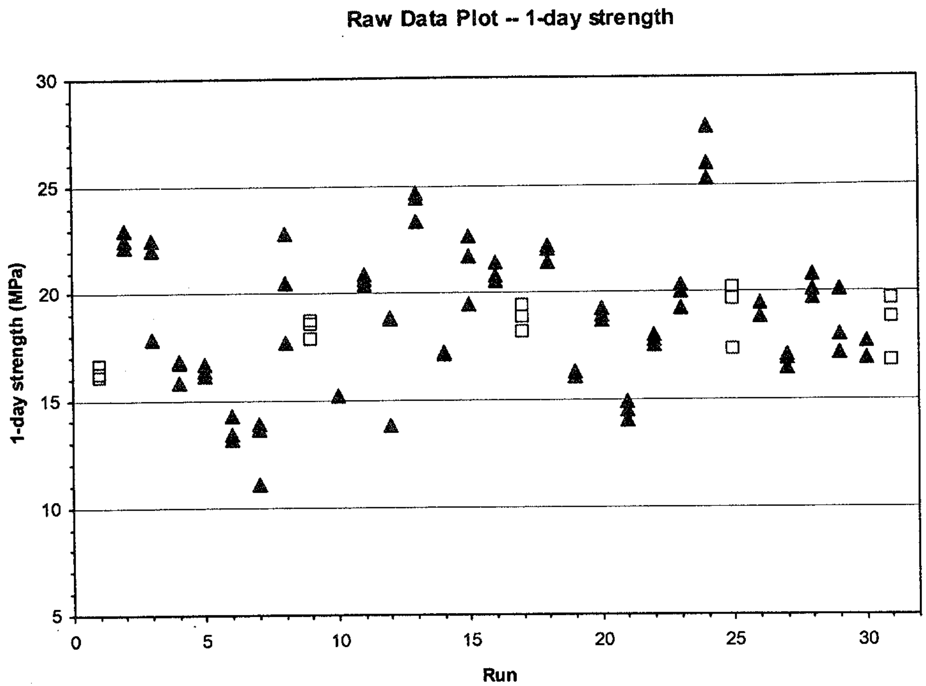


Figure 12. Raw data plot for 1-day strength (factorial experiment)

shown as hollow squares, give an indication of consistency over time. In this case, the control results are all about equal, indicating no time-related effects. Raw data plots are also helpful in identifying suspect data values, which may result from (for example) errors in data recording or data entry, equipment malfunction, or poor specimen fabrication.

Figure 13 is a scatterplot showing the effects of varying one factor (w/c) on the 1-day strength. In this case, as expected, the 1-day strength decreases with increasing w/c.

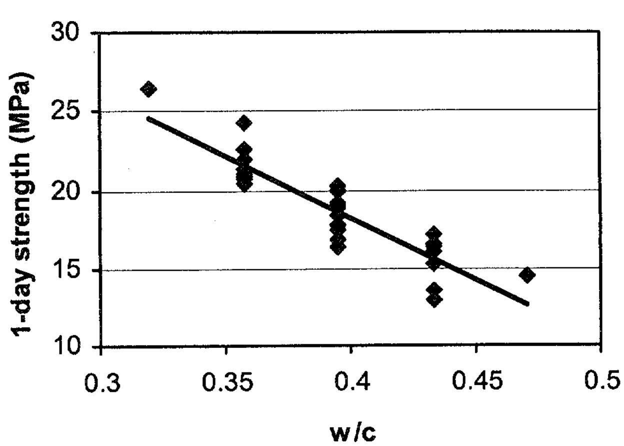


Figure 13. Scatterplot showing effect of w/c on 1-day strength (factorial experiment)

Figure 14 shows a means plot for 1-day strength. The means plot allows comparison of the effects of each factor. In this experiment, 1-day strength was clearly influenced by w/c. Other factors appear to have had little effect.

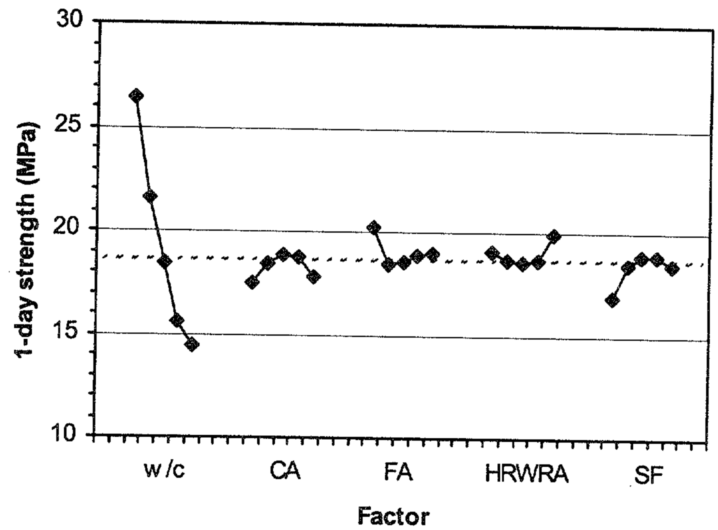


Figure 14. Means plot for 1-day strength (factorial experiment)

Finally, figure 15 shows a cube plot of 1-day strength with respect to three factors (w/c, fine aggregate, and coarse aggregate). A cube plot is a convenient means of assessing quantitative effects of three factors on a response.

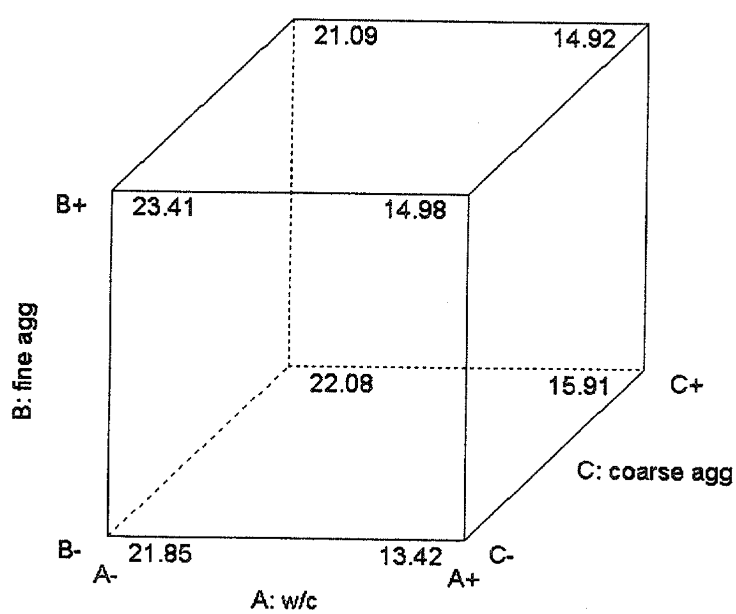


Figure 15. Example of cube plot for factorial points

4.5.3 Model Fitting and Validation for 1-Day Strength

After assessing the data graphically, the second step in analysis is to estimate an appropriate model for each response. As with the mixture approach, ANOVA and least-squares regression techniques are used. The first step is to use ANOVA to determine the appropriate type of model (e.g., linear, quadratic). An ANOVA table for sequential model sum of squares, shown in table 12, suggests that both linear and quadratic terms are significant. A lack-of-fit ANOVA table (table 13) suggests that a quadratic model has insignificant lack-of-fit ("Prob > F" = 0.8339).

Table 12. Sequential model sum of squares for 1-day strength (factorial experiment)

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	10780.54	1	10780.54	–	–
Linear	215.97	5	43.19	22.15	< 0.0001
2FI	27.35	10	2.73	1.92	0.1236
Quadratic	13.60	5	2.72	3.48	0.0441
Cubic (aliased)	1.86	5	0.37	0.31	0.8865
Residual	5.95	5	1.19	–	–
Total	11045.26	31	356.30	–	–

Table 13. Lack-of-fit test for 1-day strength (factorial experiment)

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Linear	43.98	21	2.09	1.75	0.3129
2FI	16.63	11	1.51	1.27	0.4444
Quadratic	3.03	6	0.51	0.42	0.8339
Cubic (aliased)	1.18	1	1.18	0.98	0.3772
Pure Error	4.78	4	1.19		

When a central composite design is used, the full quadratic model can be estimated, but often some of the terms are not significant. The following procedure[3] was used to identify an appropriate reduced quadratic model:

1) Fit the full quadratic model and for each coefficient, calculate the t-statistic for the null hypothesis that the coefficient is equal to zero.

2) Perform the regression again with a partial model containing only those terms that are statistically significant (i.e., those terms that had a t-statistic greater than that for the chosen

[3]This procedure may be used because the CCD experiment design is well-balanced and orthogonal (or nearly so).

significance level, in this case 0.05). Calculate the t-statistics again and drop any terms which are not significant.

3) Repeat step 2 until the partial model contains only significant terms.

4) Add first-order terms required to make the model hierarchical. Hierarchical polynomial models make sense under linear transformations such as changing units of temperature from Celsius to Fahrenheit [11]. All second-order terms that appear in the model must have corresponding first-order terms included in order to make the model hierarchical.

The ANOVA for the final hierarchical model (with the hierarchical terms shaded) is shown in table 14.

Table 14. ANOVA for 1-day strength model (factorial experiment)

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	240.87	8	30.11	27.76	< 0.0001
A	213.26	1	213.26	196.66	< 0.0001
B	0.48	1	0.48	0.45	0.5113
C	0.04	1	0.04	0.04	0.8433
E	2.06	1	2.06	1.90	0.1819
A^2	6.20	1	6.20	5.72	0.0257
AC	5.15	1	5.15	4.75	0.0404
AE	7.16	1	7.16	6.60	0.0175
BC	6.51	1	6.51	6.00	0.0227
Residual	23.86	22	1.08	–	–
Lack of fit	19.08	18	1.06	0.89	0.6248
Pure error	4.78	4	1.19	–	–
Corr. total	264.72	30	–	–	–

For one-day strength, y_2, the fitted model was:

$$\begin{aligned}\hat{y}_2 = &-63.8 - 860.8x_1 + 1361.3x_2 + 450.8x_3 - 1431.5x_5 + 323.9x_1^{\,2} + 1068x_1x_3 \\ &+ 3780x_1x_5 - 3208x_2x_3\end{aligned} \tag{17}$$

The adequacy of each fitted model was validated quantitatively by calculating statistical measures such as residual standard deviation and PRESS, and graphically by examining residual plots. The residual standard deviation, s, for this model is 0.99 MPa. A value of s near the repeatibility value (replicate standard deviation calculated from center points) is an indication of an adequately fitting model. For this experiment, the repeatibility value is 1.04 MPa, which is close to s. The PRESS statistic (see page 12) is a measure of how well the model fits each point in the design (the smaller the PRESS statistic, the better the fit). PRESS and some other quantitative indicators of model adequacy are shown in table 15.

Table 15. Summary statistics for 1-day strength model (factorial experiment)

Std. dev.	1.04
Mean	18.65
C.V.	5.58
PRESS	45.16
R-squared	0.9099
Adjusted R-squared	0.8771
Predicted R-squared	0.8294

The residuals are the deviations of the observed data values from the fitted values, x_l, and are estimates of the error terms e_i in the model. The e_i are assumed to be random and normally distributed with mean equal to zero and constant standard deviation. A normal probability plot of the residuals (shown in figure 16) is used to assess the validity of this assumption. If the error terms follow a normal distribution, they will fall on a straight line on the normal probability plot. Because they are estimates of the error terms, the residuals should exhibit similar properties.

If the assumptions are valid, plots of the residuals versus run sequence, predicted values, and other independent variables should be random and structureless. If structure remains in the residuals, residual plots may suggest modifications to the model that will remove the structure.

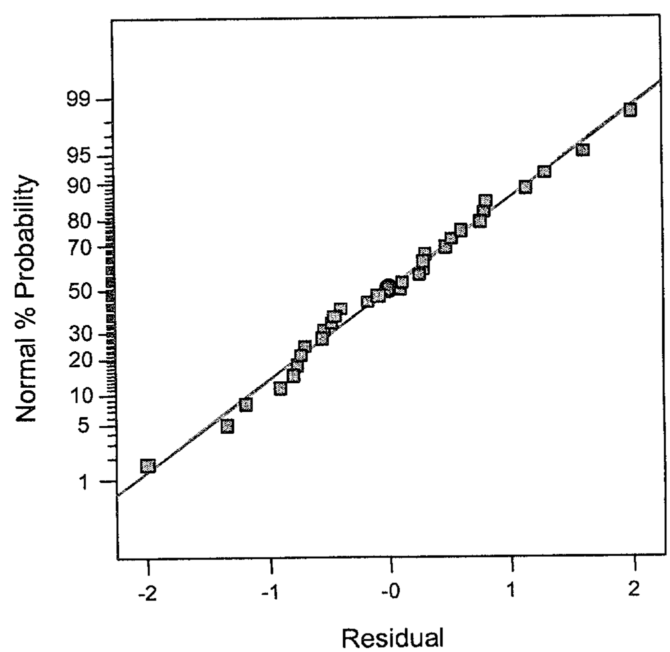


Figure 16. Example of a normal probability plot for model validation

Figure 17 shows a plot of residuals versus run sequence for 1-day strength. The plot shows no significant structure to the residuals.

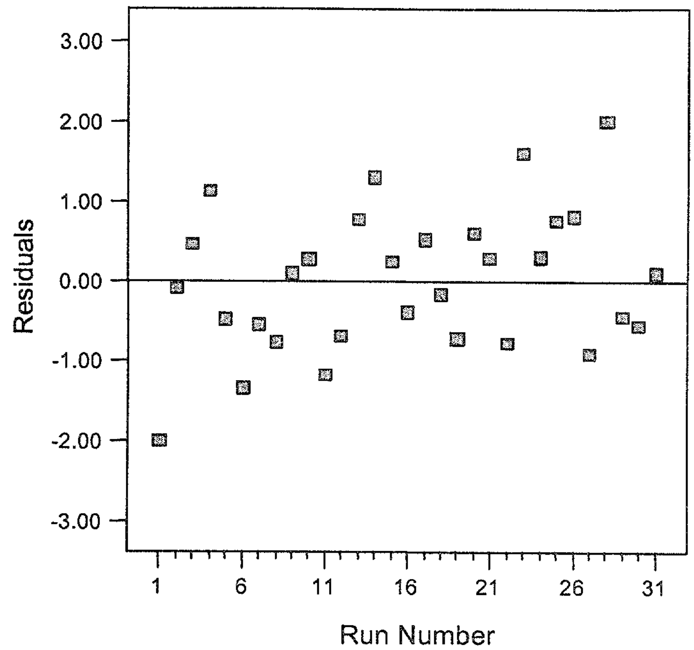


Figure 17. Example of a residual plot (residuals vs. run) for model validation

4.5.4 Models for Other Responses

Using the same procedure described above for 1-day strength, the following models were fit to slump (x_1), 28-day strength (x_3), and 42-day RCT (x_4) results:

$$\hat{y}_1 = -1365.5 - 4876.9x_1 - 8334.7x_2 + 8256.5x_3 + 6.698 \times 10^5 x_4 - 4503.6x_5 + 20185x_1x_2 - 1.564 \times 10^6 x_3x_4 \tag{18}$$

$$\hat{y}_3 = 124.0 - 227.3x_1 + 3390.0x_4 - 3937.5x_5 + 10262x_1x_5 \tag{19}$$

$$\hat{y}_4 = 635.4 + 4445.6x_1 - 1199.8x_2 - 1548.5x_3 - 31651x_5 + 1.635 \times 10^6 x_5^2 - 1.448 \times 10^5 x_1x_5 \tag{20}$$

4.6 Optimization

The objective of optimization may be to find the "best settings" (settings which maximize or minimize a particular response or responses) or to meet a set of specifications. In either case, optimization usually involves considering several responses simultaneously. The same optimization strategy that was used in the classical mixture approach can be used for a factorial approach (see chapter 3).

4.6.1 Graphical Optimization

For three or fewer responses, contour plots can be useful in identifying optimum settings. Individual contour plots can be used to identify best settings for each response. Figure 18 shows a contour plot of 28-day strength as a function of w/c and silica fume with HRWRA at its middle setting. Figure 19 shows the same plot but with HRWRA at the high setting. These plots illustrate that the highest strength is reached at the high level of HRWRA coupled with the low levels of w/c and silica fume.

Contour plots can also be overlaid with the constraints for each response defining a subarea of settings that meet the response criteria. For example, figure 20 shows all settings meeting the following criteria: RCT < 700 and slump equal 50 to 100 mm. The white area in the plot indicates the settings meeting the criteria. The gray area on the plot shows the region of settings that do not meet the constraints simultaneously. Figure 21 shows the same plot with the added constraint that 28-day strength > 51 MPa. As constraints are added, the feasible region usually gets smaller. In some situations, no settings will meet all of the criteria.

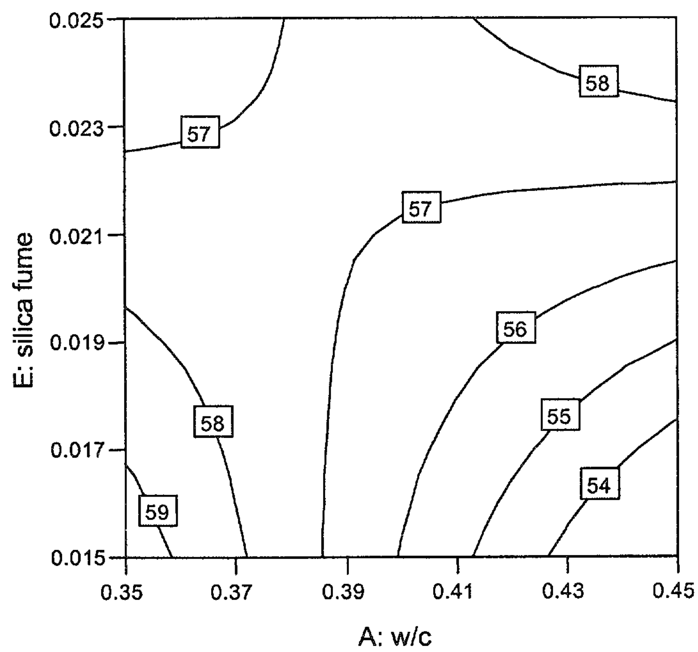


Figure 18. 28-day strength in w/c and silica fume (HRWRA at middle setting)

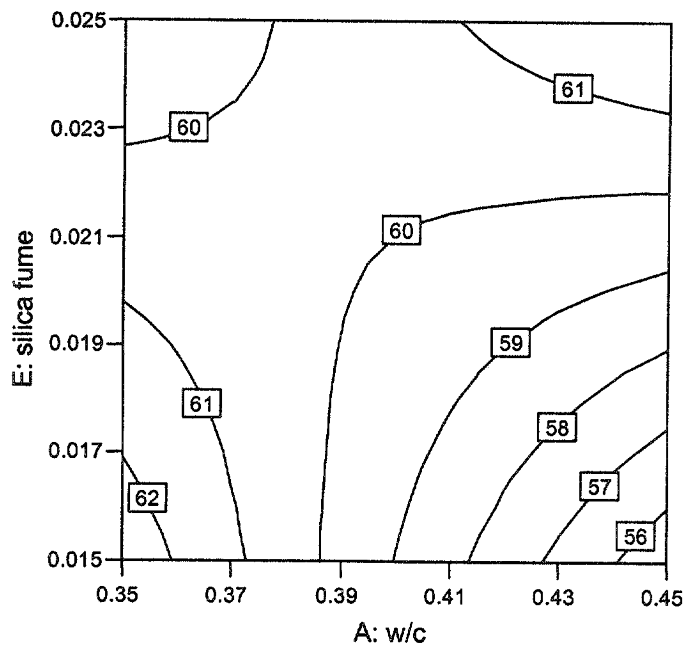


Figure 19. 28-day strength in w/c and silica fume (HRWRA at high setting)

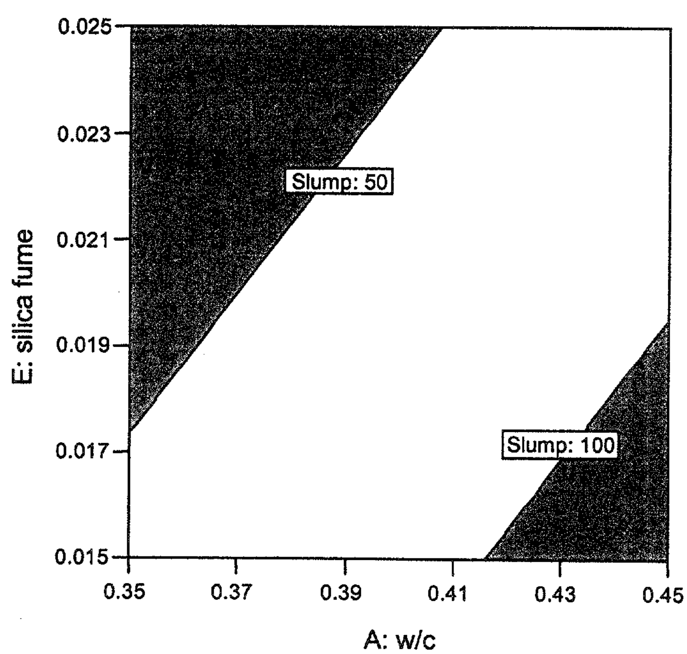


Figure 20. Overlay plot for RCT < 700 and slump = 50–100 mm

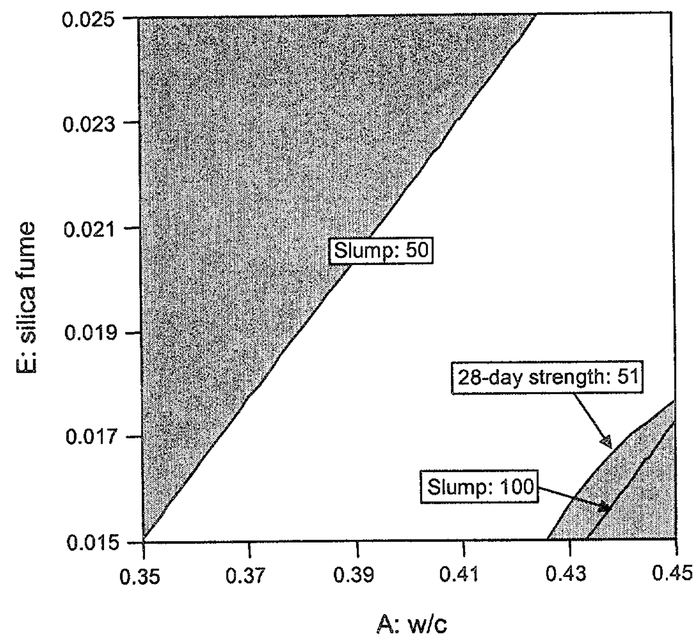


Figure 21. Overlay plot for RCT < 700, slump = 50–100 mm, and 28-day strength > 51 MPa

4.6.2 Numerical Optimization

For more than three responses considered simultaneously, numerical optimization is often more practical than graphical optimization. The numerical optimization technique using desirability functions described in chapter 2 and used in the classical mixture experiment (chapter 3) can also be applied to the factorial experiment. Desirability functions for this experiment are similar to those used in the mixture experiment, except that in some cases (e.g, cost) the endpoint values are different. The desirability functions are shown in figure 22.

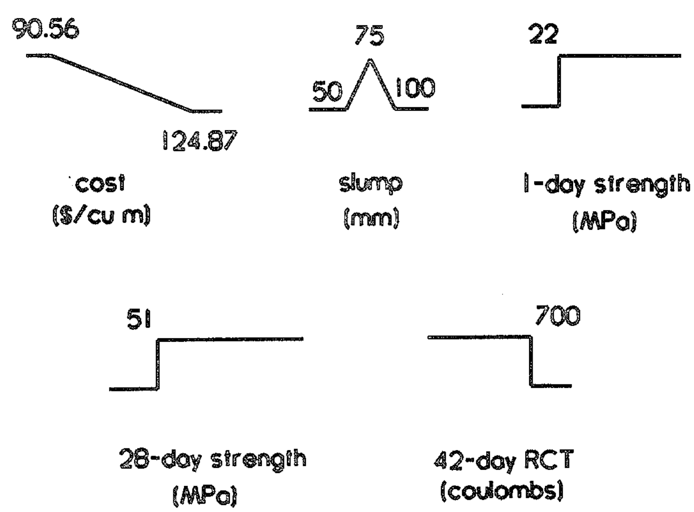


Figure 22. Desirability functions for factorial experiment

Numerical optimization gave the following best settings for this concrete mixture: w/c = 0.367 (by mass), fine aggregate volume fraction = 0.285, coarse aggregate volume fraction = 0.408, HRWRA volume fraction = 0.0061, and silica fume volume fraction = 0.0153. The predicted response values and associated uncertainties (at a 95 percent confidence level) are slump = 74 ±19 mm, 1-day strength = 22.08 ±1.17 MPa, 28-day strength = 58.65 ±2.32 MPa, and RCT = 378 ±30 coulombs, at a cost of \$100.68 per m^3.

4.6.3 Accounting for Uncertainty

As described for the mixture approach, the fitted functions (models) and values predicted from them have uncertainty associated with them because they are estimated from data. For example, for the optimal mixture proportions shown above the predicted 1-day strength is 22.08 ±1.17 MPa. If these proportions are used, we can be 95 percent confident that the true 1-day strength will lie between 20.91 and 23.25 MPa. But because the specified 1-day strength is 22 MPa, it is quite possible that the true 1-day strength will fall below the specified value. Therefore, the constraints must be modified to account for the uncertainty in the fitted functions. The uncertainties for the optimal mixture can be used to define modified constraints, and a new set of optimal mixture proportions can be identified for these new constraints. The predicted responses based on the new optimal proportions must be checked to see that the original specifications are met.

The modified constraints are slump between 69 and 81 mm, 1-day strength greater than 23.17 MPa, 28-day strength greater than 53.32 MPa, and RCT less than 670 coulombs. The best mixture for this new set of constraints is w/c = 0.358 (by mass), fine aggregate volume fraction = 0.282, coarse aggregate volume fraction = 0.4071, HRWRA volume fraction = 0.0062, and silica fume volume fraction = 0.0153. The predicted response values and associated uncertainties (at a 95 percent confidence level) are slump = 74 ±20 mm, 1-day strength = 23.17 ±1.26 MPa, 28-day strength = 59.62 ±2.68 MPa, and RCT = 363 ±32 coulombs, at a cost of \$101.65 per m^3. All but one of the lower or upper bound values for the responses now meet the original specifications. The exception is the lower bound for 1-day strength, which is 21.91 MPa (compared with the specified value of 22 MPa). In practice, this small difference is probably insignificant; however, it may be worthwhile to investigate ways to increase 1-day strength for this mix. A slightly lower w/c (0.35, for example) would probably be a sufficient remedy. The predictive models estimated from the experiment can be used to predict responses for settings anywhere within the experimental design space (i.e., anywhere within the defined variable ranges). However, extrapolation beyond the design space is not recommended.

In the factorial experiment, accounting for uncertainty increased the cost of the optimal mix only slightly (from \$100.68 to \$101.65). As with the mixture experiment, the value of optimization is evident when the cost of the optimal mix (\$101.65) is compared with the range of mixture costs in the experiment (\$90.56 to \$124.87).

CHAPTER 5
Development of Interactive Web Site (COST Program)

5.1 Introduction

The goal of the second phase of this research project was to develop an interactive Web site that can be used to optimize concrete mixture proportions using the response surface approach. The purpose of this Web site is to introduce this approach to the concrete community and to give concrete practitioners an opportunity to apply the approach to their own mixture development. Because the response surface approach was likely to be unfamiliar to many practicing engineers and producers, the aim was to make it as user-friendly as possible (within budget constraints) and to provide as much guidance as possible in interpreting results.

5.2 Selection of Approach

A systematic approach is critical when optimizing a HPC mixture subject to several performance criteria. The laboratory experiments described in chapters 3 and 4 investigated two such approaches: the classical mixture experiment design and the factorial/CCD experiment design. Using either of these approaches, a trial batch and testing program can thoroughly examine the concrete properties of interest over the selected range of component proportions, and models estimated from the data can be used to identify optimal mixes.

Using a statistical approach to mixture optimization requires a significant investment in trial batches and testing. In both the mixture approach and factorial approach, 31 different trial batches were required for a 6-component mixture. The large number of runs was required to fit a full quadratic model for each response and to provide control runs and replicate runs for estimating repeatability.

If the responses are represented adequately by linear models (as opposed to quadratic), the number of trial batches can be reduced by as much as 50 percent. In the mixture experiment (chapter 3), linear models were adequate for all but one response (1-day strength). If linear model were assumed, the number of experimental runs could have been halved. However, since materials and conditions vary by location, the quadratic model is a better initial assumption.

The factorial approach has an advantage over the mixture approach in that it can be performed sequentially (see page 10 of this report). In a sequential approach, the CCD experiment is divided into two parts. The adequacy of linear models for the responses can be assessed after the initial portion of the experiment (for a 6-component mixture, the first part would consist of 19 trial batches). If linear response models are sufficient over the range of material proportions being considered, the second part of the experiment would not be necessary. If not, the second part of the experiment can be run, and quadratic models can be fit to the data.

In both approaches, the number of runs also can be reduced by holding certain variables constant. Reducing the number of components from 6 to 4 would reduce the number of runs in a factorial/CCD experiment from 31 to 19. For example, if a user is interested primarily in a property that is influenced by cement paste characteristics, he might choose to vary only the paste component proportions while holding aggregate constant.

Based on the experimental results described in chapters 3 and 4, the two approaches, mixture and factorial, were evaluated to select the best approach for an interactive Web site. Technical suitability and practical considerations (e.g., ease of understanding, ease of use) were considered in deciding which method to use for the Web site. While both methods were considered technically suitable, the factorial approach was considered to be more practical. The advantage of sequential experimentation, which could reduce the number of required trial batches, favored the factorial approach. Furthermore, materials engineers are more likely to have encountered factorial experiments than mixture experiments, and the factorial approach is more straightforward and easier to use, understand, analyze, and interpret. Finally, the statistical software to be used for the Web site (DATAPLOT) was better suited for the factorial approach.

5.3 Considerations in Development

The following are some of the considerations that shaped the development of the COST software and Web site:

- *Introduce the response surface optimization approach in the context of concrete mixture proportioning.*

  As mentioned in chapter 1, commercially available statistical software packages can provide the required experiment design and analysis capabilities needed for this approach. However, these packages are not specifically geared toward concrete mixture proportioning. The purpose of the COST software is to introduce the RSM approach as a means of optimizing concrete mixtures. The COST software is not intended to be a state-of-the-art, all-inclusive, "definitive" software product.

- *Minimize the required number of experimental runs needed to produce an optimal mix.*

  Concrete producers want to minimize the effort (and cost) needed to identify optimal mixtures. Therefore, the maximum number of factors was limited to five, one of which is water-cement ratio or water-cementitious materials ratio. The maximum number of responses was also limited to five (one of which is cost).

- *Provide flexibility in types of component materials.*

  The most common concrete component materials were included, and in each category of material (e.g., chemical admixtures, mineral admixtures, aggregates) a "user-defined" selection was included to accommodate unusual or new materials. Flexibility was provided so a user could, for example, optimize the cementitious matrix alone (i.e., hold aggregates constant), or optimize the entire concrete mixture.

- *Recognize the limited statistical background of many potential users.*

  For this reason, guidance was included for analysis and interpretation as well as actually running the experiment. For example, potential sources of error, the importance of randomization, and the importance of accuracy in batching and in following the experimental plan are discussed. Because the results and circumstances for any user will vary widely, guidance in analysis and interpretation was limited to general aspects, such as indicating strong and weak factors. More subtle statistical analysis requires human knowledge and judgment.

- *Work within constraints associated with the use of the Web and DATAPLOT software.*

  There were several issues to contend with. Speed was one issue—the speed of transfer to and from a user's computer over the Internet to the server housing COST, and the computational speed of DATAPLOT. Computations were minimized to reduce waiting times. Speed was also an issue in generating graphics (plots). Another limitation associated with graphics was the type and quality of graphics that could be generated and presented on the Web. DATAPLOT generates postscript plots which were converted to GIF format for the Web site.

  Speed issues also prevented the use of a mathematically rigorous numerical optimization scheme. Instead, numerical optimization was achieved by calculating a score function at each point on a superimposed grid over the range of each factor. For 5 factors and 10 points per factor, this requires 10^5, or 100,000, calculations. To avoid excessive computation time, the grids were limited in size.

  In addition to speed, there were file storage, access, and privacy issues. For example, configuration and security constraints require that files be stored on the COST server. They cannot be saved on the user's computer.

5.4 Description of the Software and Web Site

5.4.1 Introduction

COST is an online interactive system developed to assist engineers, concrete producers, and researchers in optimizing portland cement concrete mixtures for their particular applications. COST applies response surface methodology (RSM), a collection of statistical experiment design and analysis methods, to the problem of optimizing concrete mixture proportions. RSM often is used in industry for product development, formulation, and improvement, and is applicable to problems such as concrete mixture proportioning where several input variables (factors) influence a performance measure (response).

COST is intended to provide an introduction to concrete practitioners who are unfamiliar with the concepts and process of applying RSM to concrete mixture proportioning. COST allows users to learn how to apply RSM to the problem of optimizing concrete mixtures.

There are two scenarios for which COST could be applied:

1. To proportion a concrete mixture to meet a set of specifications at minimum material cost. This is probably the most common scenario.

2. To maximize (or minimize) a particular response or responses, irrespective of cost.

COST can be used to optimize cement paste, mortar, or concrete mixtures. In all three cases, varying the mixture component proportions affects both fresh and hardened properties of the paste, mortar, or concrete. The properties (responses) depend on the proportions of the components.

In COST, w/c (or water-cementitious materials ratio, w/cm) is varied along with as many as four additional components. These are referred to as variable factors. Other factors may be included in the mixture at fixed (constant) levels, and are referred to as fixed factors. The user can designate as many as five concrete properties, or responses, (e.g., slump, strength, air content, cost, etc.) according to the requirements of the application.

COST is accessible via the Internet. The program consists of a front-end HTML interface that allows the user to enter required information. Underlying code (written in C) processes the input, generates the experiment designs and mixture proportions, calls routines for statistical analysis, and generates output. The statistical analysis routines are part of an interactive statistical software package, DATAPLOT, which was developed at NIST. COST is not intended to supplant or compete with commercially available experiment design and analysis software packages. Rather, COST's purpose is to introduce to the concrete practitioner the concepts of statistical experiment design and analysis using RSM and to explain how these concepts might be applied to concrete mixture proportioning. COST is specifically geared toward applying these methods to concrete mixture proportioning.

This section provides a brief, general overview of COST. The COST User's Guide, which describes the step-by-step approach of the Web site, is included as appendix C of this report.

5.4.2 Overview of COST Six-Step Process

The tasks required to optimize a concrete mixture using statistical methods have been assigned to the six steps listed below:

- Specify responses.
- Specify mixtures.
- Run trial batches.
- Enter results.
- Analyze data.
- Summarize analysis.

In most cases, these steps will be performed in the order listed above. Each step is described in detail in the COST User's Guide (see appendix C).

Before starting the six-step process, the user should define the overall objective of the project. Typical objectives include the following:

- Minimize cost while meeting several performance criteria for responses.
- Minimize or maximize a single response or several responses.

Step 1: Specify Responses

The first step is to specify the responses of interest. Responses are the concrete properties which the user is interested in, and are usually dictated by job requirements. The units (e.g., MPa, mm) and the allowable range of the response must also be specified. The allowable range defines the performance specification for the response. For example, a response like slump may have an allowable range between 50 and 100 mm. Another response, like strength, may have a specified minimum value greater than 40 MPa.

Step 2: Specify Mixtures

Step 2 involves specifying the concrete mixture components and their ranges. Concrete may contain a variety of component materials. Allowable material types for this version of COST include the following:

- Water.[1]
- Cement.[1]
- Mineral admixtures (up to 4): fly ash, silica fume, slag, other (user specified).
- Chemical admixtures (up to 3): all user specified.
- Aggregates (up to 3): coarse, fine, other (user specified).

Each component, or factor, may be variable or fixed (set at a constant level). For concrete mixture proportioning, variable factors would usually be the mixture components expected to have the most significant effects on the responses. Fixed factors would be those expected to have little or no effect on the responses, allowing them to be held constant in the experiment. Any of the components included in COST may be set as variable or fixed; however, COST limits the user to a maximum of five variable factors for any one experiment (the greater the number of variable factors, the greater the number of trial batches required). Because w/c or w/cm is always considered to be one factor, as many as six material components (water, cement, and four others) may be varied.

The user must also provide information about material properties (e.g., for cement, specific gravity) and costs for each component to be included. Details on property information required can be found in the COST User's Guide (appendix C).

---

[1]Water and cement are entered in terms of w/c or w/cm. COST always requires that either w/c or w/cm be included as a variable factor. Thus, the two mixture components, water and cement, are accounted for in one factor.

After the user has decided which factors to include, defined their ranges (for variable factors) or constant levels (for fixed factors), and entered required material information into the COST program, a trial batch plan is generated.

Step 3: Running the Experiment

After generating a trial batch plan, the next step is to perform the experiment. The experiment in this case is a set of trial batches from which specimens will be fabricated and tested for the responses specified in Step 1.

Step 4: Enter Results

After testing is completed, the test results are input into COST for analysis. The data are entered into a form, which is set up according to the experimental plan.

Step 5: Analyze Results

Analysis of the results consists of 10 tasks, which are performed using one or more statistical tools. Table 16 summarizes these analyses. The analysis techniques employed by COST consist of both graphical analysis and numerical analysis (modeling), which can be classified in the following groups:

- Quantitative description of data—task 1.
- Assessing the experiment design—tasks 2, 3, 4.
- Graphical description of data—tasks 5, 6.
- Optimization (determining best settings)—tasks 7, 8, 9, 10.

Examples and details on each analysis task can be found in the COST User's Guide (appendix C).

Step 6: Summarize Analysis

The final step summarizes the analysis. The summary includes a list of the component variables, the responses, and the optimum settings based on three different perspectives: mean values, individual runs, and numerical optimization. A sample of the summary screen is shown in figure 23.

Table 16. Summary of analysis tasks and tools in COST

Task #	Task Description	Tool(s)
1	Characterize response variables	Summary statistics
2	Assess balance of design	Counts plot matrix
3	Assess optimality of design points—all responses jointly	Counts in admissible region matrix Percentage in admissible region plots
4	Assess optimality of design points—all four responses jointly	Percentage in admissible region plots
5	Determine interrelationships between responses	Scatterplots of response variables Scatterplots of response variables vs. factors
6	Assess relationship between response variables and factors	Means plots of responses vs. factors
7	Determine optimal settings for each factor	Best settings based on mean values Best settings based on individual runs
8	Model fitting and verification	Model fitting tool
9	Numerical optimization	Best settings based on maximum total score
10	Response prediction	Response prediction tool

Variables examined:

`w/c_ratio`   `fine_agg`   `coarse_agg`   `HRWRA`   `Silica_fume`

Responses evaluated:

`Cost`   `Slump`   `1-day_Str`   `28-day_Str`   `RCT`

Optimum Settings

Units are the same as those used in the specify mixtures form previously

Aggregates are in terms of volume or mass fraction (as previously selected by user)

Mineral admixtures are in terms of percent cement mass replacement

Chemical admixtures are in terms of liters per kg of cement

Variable	Mean Values Optimum setting	Individual Runs Optimum setting	Numerical Optimization Optimum setting
w/c_ratio	0.3200	0.3576	0.3576
fine_agg	0.2853	0.2853	0.2712
coarse_agg	0.4353	0.4353	0.4071
HRWRA	0.0051	0.0051	0.0051
Silica_fume	0.0294	0.0247	0.0228

Figure 23. Summary screen from COST

5.5 Future Considerations

The current version of COST, while functional, is limited in several respects, because it is Web-based software and because of the specific architecture involved. The software runs slowly, the graphical capabilities are limited, and data is stored on the host computer instead of the user's computer. A stand-alone, Microsoft® Windows®-based version of COST could be developed in the future. However, there are commercially available statistical software packages that could be used for this application. Because these packages are general in nature (i.e., not specifically geared towards concrete mixture proportioning), some care is needed to assure that they are being used correctly.

ACKNOWLEDGMENTS

Eric S. Lagergren (Nabisco Research) provided valuable assistance in developing the experiment designs for the laboratory experiments and analyzing the experimental results.

James J. Filliben (NIST) assisted in developing experiment designs for the laboratory work and provided experiment design, data analysis and DATAPLOT expertise in the development of the COST Web site software.

Dale Bentz (NIST) programmed the COST Web site software and provided concrete materials expertise to the Web site development process.

Leif Wathne (SaLUT, Inc.) assisted in planning the experiments and supervised the laboratory work.

Joseph Brookman, Brian Goril, and Felix Okoye (formerly of SaLUT, Inc.), performed the laboratory work.

Ken Snyder (NIST) performed rapid chloride testing for Phase I of the laboratory work.

The "COST User's Guide" (appendix C) was written by Marcia Simon, Dale Bentz, and Jim Filliben.

REFERENCES

1. Rougeron, P. and P.C. Aitcin, "Optimization of the Composition of a High-Performance Concrete," *Cement, Concrete and Aggregates*, V. 16, No. 2, December, 1994, pp. 115-124.

2. ACI Committee 211, "Standard Practice for Selecting Proportions for Normal, Heavyweight, and Mass Concrete." In *ACI Manual of Concrete Practice,* Volume 1. Detroit: American Concrete Institute, 1995.

3. Myers, R.H. and D.C. Montgomery. *Response Surface Methodology: Process and Product Optimization Using Designed Experiment*s, New York: Wiley, 1995.

4. Luciano, J.J, Nmai, C.K., and J.R. DelGado, "A Novel Approach to Developing High-Strength Concrete," *Concrete International*, May, 1991, pp. 25-29.

5. Bajorski, P., Streeter, D.A., and R.J. Perry, "Applying Statistical Methods for Further Improvement of High-Performance Concrete for New York State Bridge Decks," *Transportation Research Record No. 1574*, Transportation Research Board, Washington, DC, 1997, pp. 71-79.

6. DeLarrard, F., and A. Belloc, "The Influence of Aggregate on the Compressive Strength of Normal and High-Strength Concrete." *ACI Materials Journal*, V. 94, No. 5, 1997, pp. 417-426.

7. Cornell, *How to Run Mixture Experiments for Product Quality*, American Society for Quality Control, 1990.

8. Piepel and Cornell, "Mixture Experiment Approaches: Examples, Discussion, and Recommendations." *Journal of Quality Technology*, Vol. 26, No. 3, July, 1994, pp. 177-196.

9. Box, G.E.P, Hunter, W.G., and J.S. Hunter, *Statistics for Experimenters*, New York: Wiley, 1978.

10. Derringer, G. and R. Suich, "Simultaneous Optimization of Several Response Variables," *Journal of Quality Technology*, Vol. 12, No. 4, October, 1980, pp. 214-219.

11. Peixoto, J. L., "Hierarchical Variable Selection in Polynomial Regression Models," *The American Statistician*, Vol. 41, No. 4, November, 1987.

12. *Design Expert 6 User's Guide*, Stat-Ease, Inc., Minneapolis, MN, 2000.

APPENDIX A. Experiment Design and Data Analysis for Mixture Experiment

A.1 Experiment Design and Response Data

Table A-1. Mixture experiment design in terms of volume fractions of components

Standard Order	Design ID	Run Order	A Water	B Cement	C Silica Fume	D HRWRA	E Coarse Agg	F Fine Agg
35	127	1	0.1720	0.1395	0.0130	0.0060	0.4098	0.2598
7	15	2	0.1656	0.1500	0.0270	0.0074	0.4000	0.2500
14	38	3	0.1767	0.1417	0.0270	0.0046	0.4000	0.2500
11	22	4	0.1850	0.1474	0.0130	0.0046	0.4000	0.2500
22	71	5	0.1600	0.1500	0.0130	0.0074	0.4098	0.2598
4	11	6	0.1850	0.1300	0.0130	0.0046	0.4174	0.2500
2	5	7	0.1600	0.1300	0.0270	0.0046	0.4284	0.2500
8	16	8	0.1600	0.1300	0.0130	0.0046	0.4424	0.2500
27	91	9	0.1850	0.1300	0.0130	0.0074	0.4073	0.2573
29	101	10	0.1712	0.1500	0.0130	0.0046	0.4112	0.2500
24	78	11	0.1850	0.1300	0.0270	0.0074	0.4003	0.2503
37	127	12	0.1720	0.1395	0.0130	0.0060	0.4098	0.2598
9	20	13	0.1850	0.1300	0.0130	0.0046	0.4000	0.2674
30	103	14	0.1600	0.1500	0.0130	0.0060	0.4210	0.2500
5	13	15	0.1600	0.1300	0.0130	0.0046	0.4000	0.2924
12	28	16	0.1600	0.1300	0.0270	0.0046	0.4000	0.2784
28	98	17	0.1600	0.1400	0.0130	0.0046	0.4324	0.2500
36	127	18	0.1720	0.1395	0.0130	0.0060	0.4098	0.2598
26	89	19	0.1600	0.1400	0.0130	0.0046	0.4000	0.2824
39	163	20	0.1656	0.1343	0.0165	0.0067	0.4234	0.2536
31	110	21	0.1712	0.1500	0.0130	0.0046	0.4000	0.2612
1	5	22	0.1600	0.1300	0.0270	0.0046	0.4284	0.2500
3	11	23	0.1850	0.1300	0.0130	0.0046	0.4174	0.2500
25	87	24	0.1600	0.1300	0.0130	0.0046	0.4212	0.2712
20	66	25	0.1600	0.1300	0.0270	0.0074	0.4128	0.2628
16	38	26	0.1767	0.1417	0.0270	0.0046	0.4000	0.2500
18	63	27	0.1725	0.1300	0.0270	0.0074	0.4131	0.2500
17	48	28	0.1725	0.1300	0.0130	0.0074	0.4000	0.2771
21	70	29	0.1600	0.1500	0.0130	0.0060	0.4000	0.2710
13	37	30	0.1600	0.1400	0.0270	0.0074	0.4000	0.2656
19	65	31	0.1600	0.1400	0.0270	0.0074	0.4156	0.2500
38	127	32	0.1720	0.1395	0.0130	0.0060	0.4098	0.2598
32	116	33	0.1725	0.1300	0.0270	0.0074	0.4000	0.2631
10	20	34	0.1850	0.1300	0.0130	0.0046	0.4000	0.2674
23	71	35	0.1600	0.1500	0.0130	0.0074	0.4098	0.2598
33	123	36	0.1600	0.1400	0.0200	0.0060	0.4120	0.2620
34	127	37	0.1720	0.1395	0.0130	0.0060	0.4098	0.2598
6	15	38	0.1656	0.1500	0.0270	0.0074	0.4000	0.2500
15	38	39	0.1767	0.1417	0.0270	0.0046	0.4000	0.2500

Table A-2. Mixture experiment: slump and 1-day strength data

Obs	Design ID	Run Order	Slump (mm)		1-Day Strength (MPa)			
32	127	1	50.8	54.0	24.3	24.4	24.0	–
6	15	2	25.4	31.8	24.6	22.9	25.9	–
13	38	3	19.1	19.1	22.7	22.6	22.1	–
10	22	4	69.9	63.5	21.1	21.4	21.8	–
20	71	5	63.5	50.8	26.9	27.2	26.5	27.5
3	11	6	108.0	95.3	16.7	16.6	17.0	–
1	5	7	12.7	12.7	21.7	23.3	22.2	–
7	16	8	38.1	31.8	21.8	21.6	21.4	–
25	91	9	203.2	196.9	17.1	16.6	16.7	–
27	101	10	25.4	19.1	26.4	26.5	26.8	–
22	78	11	127.0	127.0	19.2	19.3	19.0	–
33	127	12	101.6	95.3	20.8	21.9	21.9	–
8	20	13	114.3	120.7	18.3	18.0	18.3	–
28	103	14	63.5	63.5	28.0	26.8	27.3	–
5	13	15	63.5	50.8	22.7	21.7	21.0	–
11	28	16	31.8	25.4	21.1	22.9	22.5	–
26	98	17	31.8	31.8	25.2	26.4	24.2	–
34	127	18	95.3	88.9	21.5	21.6	23.8	–
24	89	19	38.1	38.1	18.1	23.1	24.0	–
36	163	20	95.3	95.3	22.1	21.6	22.4	–
29	110	21	50.8	50.8	24.5	25.1	24.4	–
2	5	22	25.4	25.4	22.1	24.0	24.2	–
4	11	23	114.3	114.3	17.1	16.5	15.9	–
23	87	24	63.5	69.9	24.9	20.6	23.2	–
18	66	25	76.2	76.2	25.0	24.1	25.1	–
14	38	26	31.8	25.4	22.9	23.6	22.5	–
16	63	27	101.6	95.3	21.6	22.0	21.4	–
15	48	28	177.8	165.1	22.7	22.7	23.7	–
19	70	29	50.8	50.8	27.5	27.3	27.6	–
12	37	30	38.1	31.8	26.8	27.8	27.4	–
17	65	31	31.8	31.8	28.6	25.5	27.6	–
35	127	32	120.7	120.7	22.9	22.2	22.1	–
30	116	33	114.3	114.3	23.9	23.7	24.1	–
9	20	34	127.0	127.0	18.8	18.6	18.5	–
21	71	35	114.3	101.6	29.5	28.0	28.9	–
31	123	36	76.2	69.9	26.2	26.4	27.3	–
32	127	37	101.6	101.6	23.9	24.3	24.2	–
6	15	38	50.8	50.8	29.2	27.6	29.5	–
13	38	39	25.4	25.4	23.3	25.4	22.2	–

Table A-3. Mixture experiment: 28-day strength and RCT charge passed data

Obs	Design ID	Run Order	28-Day Strength (psi)				RCT Charge Passed (coulombs)		
32	127	1	51.0	52.5	54.9	–	–	–	–
6	15	2	59.4	58.7	59.5	–	–	–	–
13	38	3	50.8	50.1	52.7	–	–	–	–
10	22	4	47.9	48.0	48.8	–	1203	1310	1321
20	71	5	51.9	56.7	57.0	–	901	790	894
3	11	6	47.3	51.7	46.6	–	1141	1308	1038
1	5	7	46.1	49.4	49.9	–	422	352	–
7	16	8	54.6	53.2	51.5	–	708	–	843
25	91	9	58.8	60.4	62.1	–	1092	1113	877
27	101	10	57.0	52.3	51.6	–	730	736	767
22	78	11	51.0	55.4	48.6	–	474	454	549
33	127	12	51.1	52.3	47.4	–	853	885	789
8	20	13	51.9	50.2	50.7	–	995	922	793
28	103	14	60.4	56.6	46.2	55.1	607	576	565
5	13	15	51.0	55.6	52.8	–	575	719	758
11	28	16	56.5	50.8	53.4	–	327	268	282
26	98	17	55.5	50.5	49.8	–	580	579	653
34	127	18	53.7	54.2	54.3	–	841	852	848
24	89	19	52.6	58.3	50.2	56.3	677	656	826
36	163	20	61.1	61.0	60.2	–	544	552	566
29	110	21	52.3	52.9	54.4	–	716	804	857
2	5	22	56.3	52.0	53.9	–	308	441	296
4	11	23	49.2	47.8	46.9	–	894	1054	956
23	87	24	53.0	50.4	49.4	–	751	618	732
18	66	25	57.1	62.6	59.7	–	326	319	303
14	38	26	57.4	51.8	50.3	–	450	346	375
16	63	27	56.6	54.5	54.5	–	324	324	257
15	48	28	58.9	58.0	57.3	–	622	702	723
19	70	29	54.7	52.5	56.4	–	496	494	524
12	37	30	49.2	57.8	59.7	57.4	247	254	234
17	65	31	53.5	49.1	50.8	–	285	350	296
35	127	32	57.8	58.6	55.0	–	661	567	680
30	116	33	57.8	57.3	53.5	–	367	358	343
9	20	34	51.1	51.9	51.9	–	804	901	754
21	71	35	64.9	65.6	65.2	–	550	566	543
31	123	36	61.5	59.8	61.8	–	318	312	390
32	127	37	53.8	55.4	54.6	–	640	614	665
6	15	38	61.6	57.5	55.2	–	235	232	250
13	38	39	54.5	53.8	55.4	–	323	379	293

A.2 Data Analysis and Model Fitting

A.2.1 Slump

Table A-4. Mixture experiment: sequential model sum of squares for slump

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	212697.8	1	212697.8	–	–
Linear	62543.72	5	12508.74	45.64	< 0.0001
Quadratic	4107.07	15	273.80	1.00	0.5016
Special cubic (aliased)	2164.86	7	309.27	1.27	0.3703
Cubic (aliased)	0.00	0		–	–
Residual	1950.91	8	243.86	–	–
Total	283464.3	36	7874.01	–	–

Table A-5. Mixture experiment: lack-of-fit test for slump

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Linear	6271.93	22	285.09	1.17	0.4335
Quadratic	2164.86	7	309.27	1.27	0.3703
Special cubic (aliased)	0.00	0	–	–	–
Cubic (aliased)	0.00	0	–	–	–
Pure error	1950.91	8	243.86	–	–

Table A-6. Mixture experiment: model summary statistics for slump

Source	Std. Dev.	r^2	Adj. r^2	Pred. r^2	PRESS
Linear	16.56	0.8838	0.8644	0.8407	11272.43
Quadratic	16.56	0.9418	0.8643	0.6049	27956.70
Special cubic (aliased)	15.62	0.9724	0.8794	–	undefined
Cubic (aliased)	–	–	–	–	undefined

Table A-7. Mixture experiment: ANOVA for slump mixture model

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	62543.72	5	12508.74	45.64	< 0.0001
Linear mixture	62543.72	5	12508.74	45.64	< 0.0001
Residual	8222.84	30	274.09	–	–
Lack of fit	6271.93	22	285.09	1.17	0.4335
Pure error	1950.91	8	243.86	–	–
Corrected total	70766.56	35	–	–	–

Table A-8. Mixture experiment: coefficient estimates for slump mixture model

Component	Coeff. Estimate	DF	Std. Error	95% CI Low	95% CI High
Water	155.68	1	10.12	135.03	176.34
Cement	–37.53	1	13.34	–64.77	–10.30
Silica fume	–80.39	1	17.95	–117.04	–43.74
HRWRA	1092.78	1	100.02	888.51	1297.04
Coarse aggregate	55.14	1	8.85	37.07	73.22
Fine aggregate	71.03	1	9.29	52.06	90.00

Table A-9. Mixture experiment: adjusted effects for slump mixture model

Component	Adjusted Effect	DF	Std. Error	Approx. t for H_o Effect = 0	Prob > t
Water	–138.04	1	12.96	–2.94	0.0063
Cement	–139.80	1	12.43	–11.25	< 0.0001
Silica fume	–114.84	1	10.42	–11.02	< 0.0001
HRWRA	70.00	1	6.83	10.25	< 0.0001
Coarse aggregate	–185.17	1	20.68	–8.95	< 0.0001
Fine aggregate	–166.11	1	22.02	–7.54	< 0.0001

Model equation in terms of pseudocomponents:

Slump = 155.68*A – 37.53*B – 80.39*C + 1092.78*D + 55.14*E + 71.03*F

Model equation in terms of real components:

Slump = 2166.5*water – 2390.5*cement – 3401.2*silica fume + 24267.7*HRWRA
– 204.8*Coarse agg +169.9*Fine agg

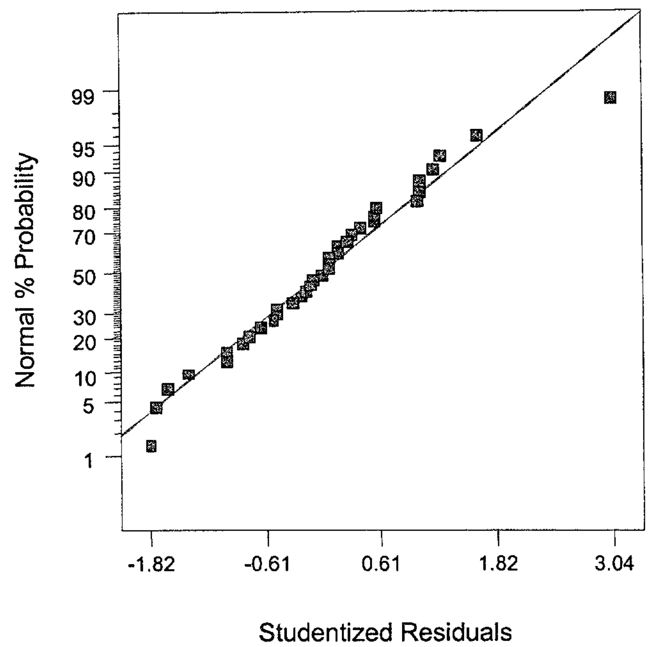


Figure A-1. Mixture experiment: normal probability plot for slump

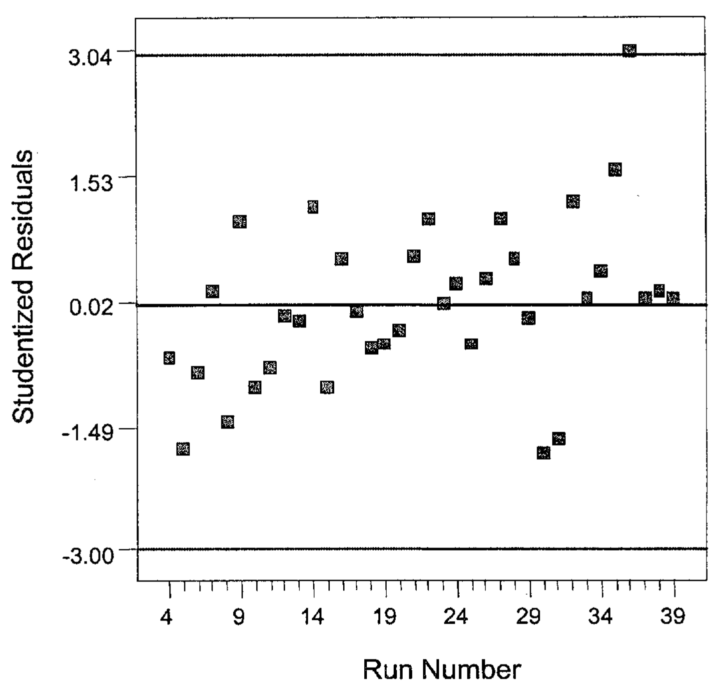


Figure A-2. Mixture experiment: residuals vs. run for slump

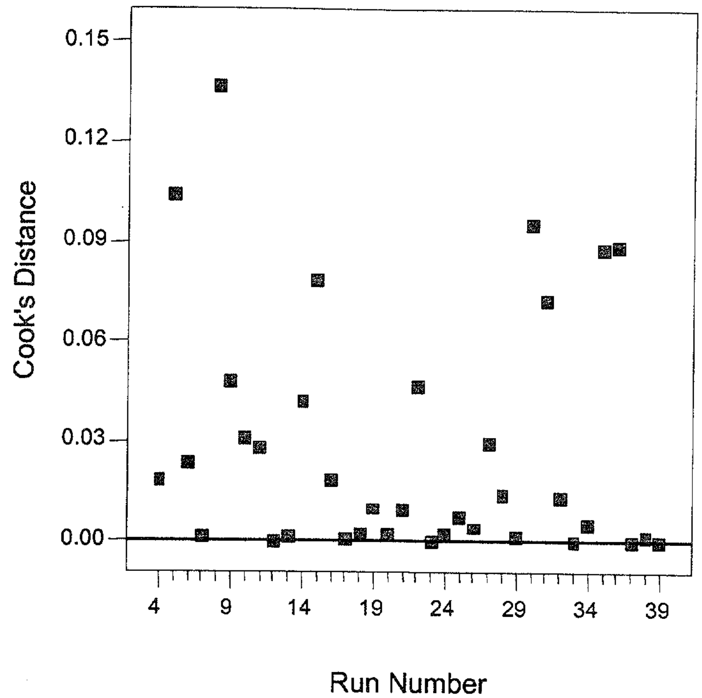


Figure A-3. Mixture experiment: Cook's distance for slump

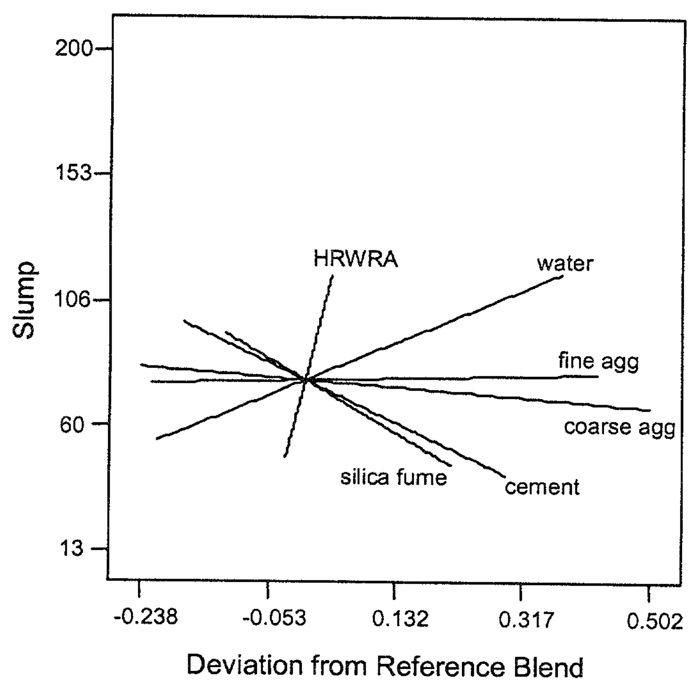


Figure A-4. Mixture experiment: trace plot for slump

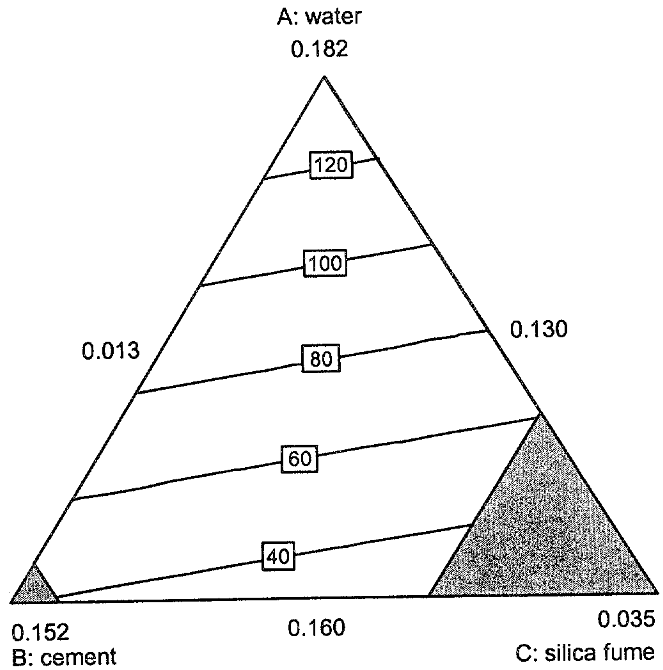


Figure A-5. Mixture experiment: contour plot for slump in water, cement, and silica fume

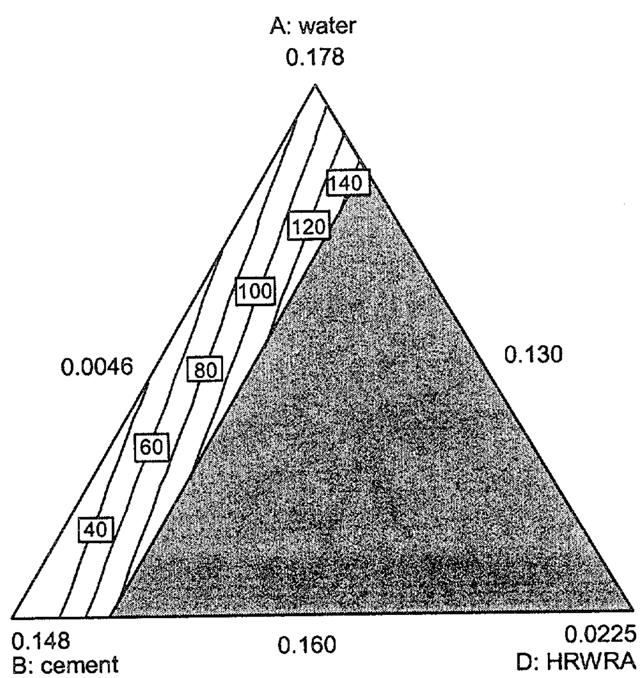


Figure A-6. Mixture experiment: contour plot of slump in water, cement, and HRWRA

A.2.2 1-Day Strength

Table A-10. Mixture experiment: sequential model sum of squares for 1-day strength

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	19278.40	1	19278.40	–	–
Linear	351.33	5	70.27	57.34	< 0.0001
Quadratic	27.14	15	1.81	2.82	0.0266
Special cubic (aliased)	3.43	7	0.49	0.63	0.7199
Cubic (aliased)	0.00	0	–	–	–
Residual	6.19	8	0.77	–	–
Total	19666.48	36	546.29	–	–

Table A-11. Mixture experiment: lack-of-fit test for 1-day strength

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Linear	30.57	22	1.39	1.79	0.1992
Quadratic	3.43	7	0.49	0.63	0.7199
Special cubic (aliased)	0.000	0	–	–	–
Cubic (aliased)	0.000	0	–	–	–
Pure error	6.19	8	0.77	–	–

Table A-12. Mixture experiment: summary statistics for 1-day strength

Source	Std. Dev.	r^2	Adj. r^2	Pred. r^2	PRESS
Linear	1.11	0.9053	0.8895	0.8611	53.89
Quadratic	0.80	0.9752	0.9421	0.8566	55.65
Special cubic (aliased)	0.88	0.9840	0.9302	–	undefined
Cubic (aliased)	–	–	–	–	undefined

Table A-13. Mixture experiment: ANOVA for 1-day strength mixture model

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	373.09	9	41.45	71.84	< 0.0001
Linear mixture	351.77	5	70.35	121.93	< 0.0001
AF	4.14	1	4.14	7.18	0.0126
BF	5.38	1	5.38	9.32	0.0052
CD	3.96	1	3.96	6.86	0.0145
DF	7.83	1	7.83	13.58	0.0011
Residual	15.00	26	0.58	–	–
Lack of fit	8.81	18	0.49	0.63	0.8010
Pure error	6.19	8	0.77	–	–
Corrected total	388.09	35	–	–	–

Table A-14. Mixture experiment: coefficient estimates for 1-day strength mixture model

Component	Coeff. Estimate	DF	Std. Error	95% CI Low	95% CI High
water	12.93	1	0.62	11.64	14.21
Cement	35.42	1	0.83	33.72	37.12
Silica fume	24.89	1	1.15	22.52	27.25
HRWRA	10.83	1	8.88	-7.42	29.07
Coarse aggregate	22.04	1	0.43	21.16	22.93
Fine aggregate	21.50	1	0.57	20.32	22.67
Water—fine aggregate	7.58	1	2.83	1.77	13.39
Cement—fine aggregate	-10.07	1	3.30	-16.86	-3.29
Silica fume—HRWRA	78.71	1	30.04	16.95	140.47
HRWRA—fine aggregate	80.50	1	21.85	35.60	125.41

Model equation in terms of pseudocomponents:

$$\text{Slump} = 12.93*A + 35.42*B + 24.89*C + 10.83*D + 22.04*E + 21.50*F + 7.58*A*F - 10.07*B*F + 78.71*C*D + 80.50*D*F$$

Model equation in terms of real components:

$$\begin{aligned}\text{Slump} = \; & -1209.1*\text{water} + 1775.9*\text{cement} - 74.71*\text{SF} - 11969*\text{HRWRA} \\ & + 59.59*\text{Coarse agg} - 105.24*\text{Fine agg} + 4214.9*\text{water}*\text{Fine agg} \\ & - 5603.1*\text{cement}*\text{Fine agg} + 43782*\text{SF}*\text{HRWRA} + 44781*\text{HRWRA}*\text{Fine agg}\end{aligned}$$

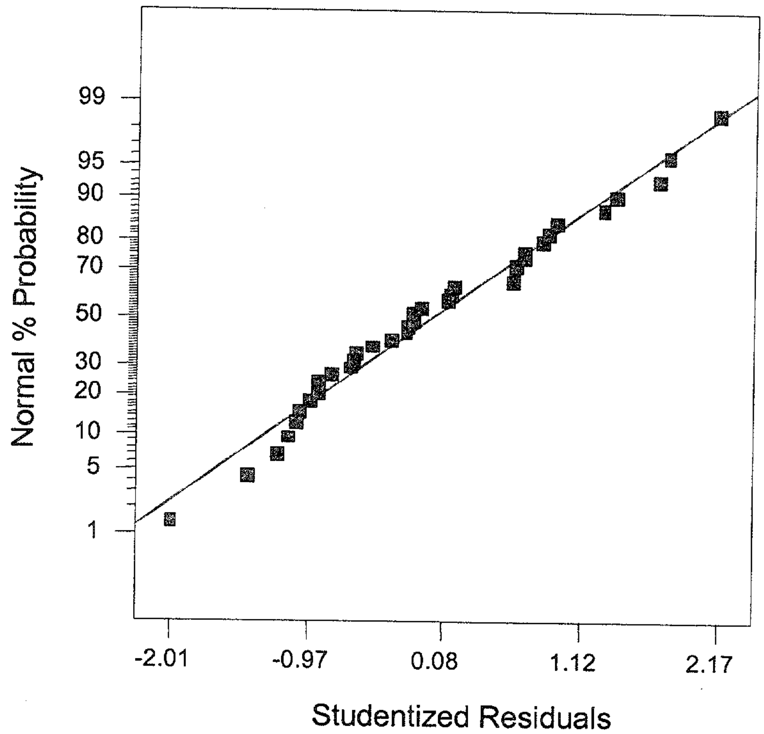


Figure A-7. Mixture experiment: normal probability plot for 1-day strength

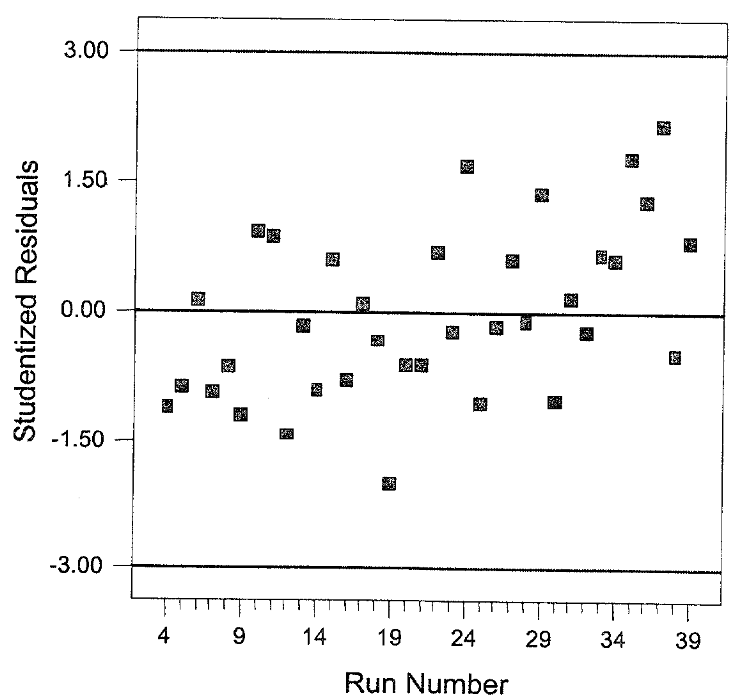


Figure A-8. Mixture experiment: residuals vs. run for 1-day strength

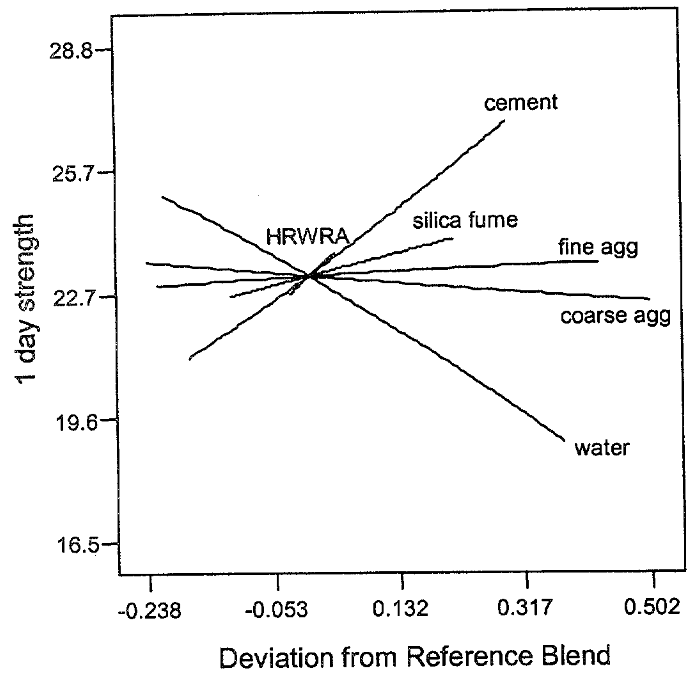


Figure A-9. Mixture experiment: trace plot for 1-day strength

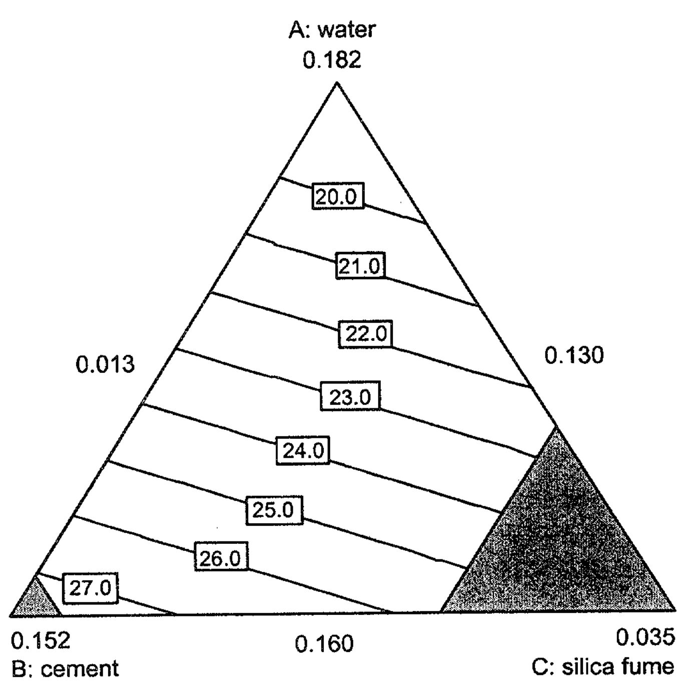


Figure A-10. Mixture experiment: contour plot of 1-day strength in water, cement, and silica fume

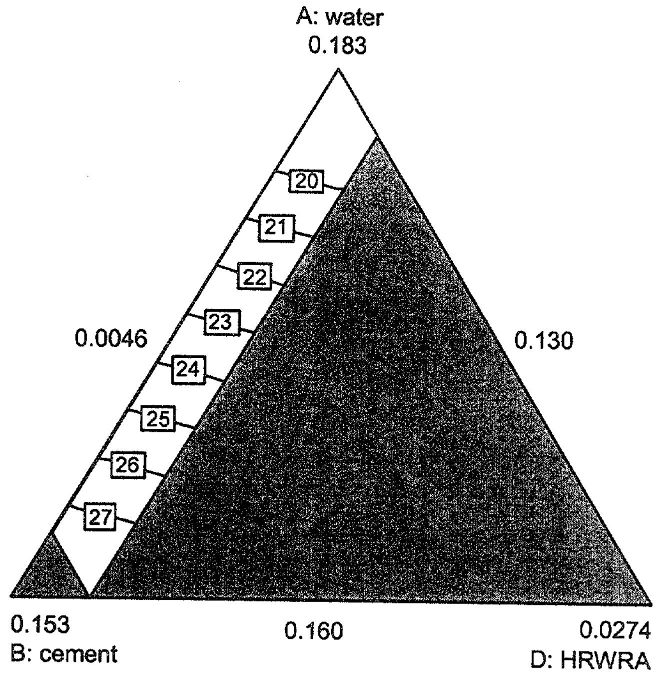


Figure A-11. Mixture experiment: contour plot of 1-day strength in water, cement, and HRWRA

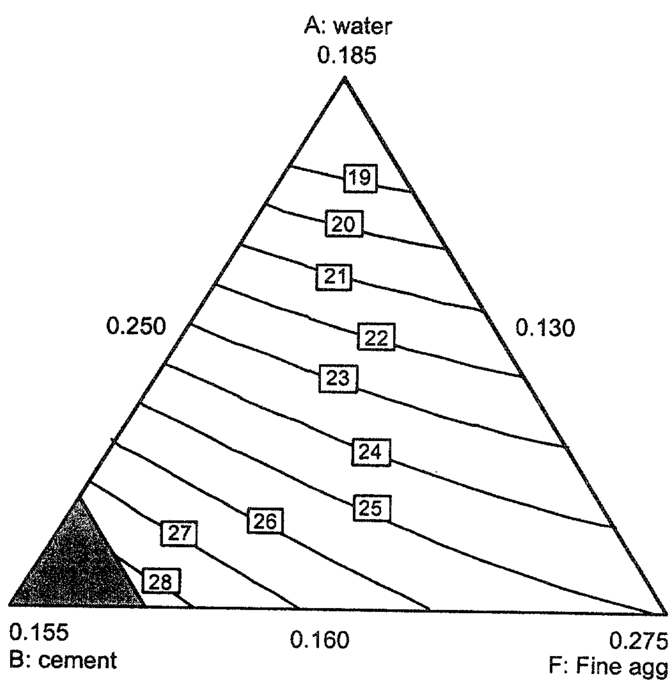


Figure A-12. Mixture experiment: contour plot of 1-day strength in water, cement, and fine aggregate

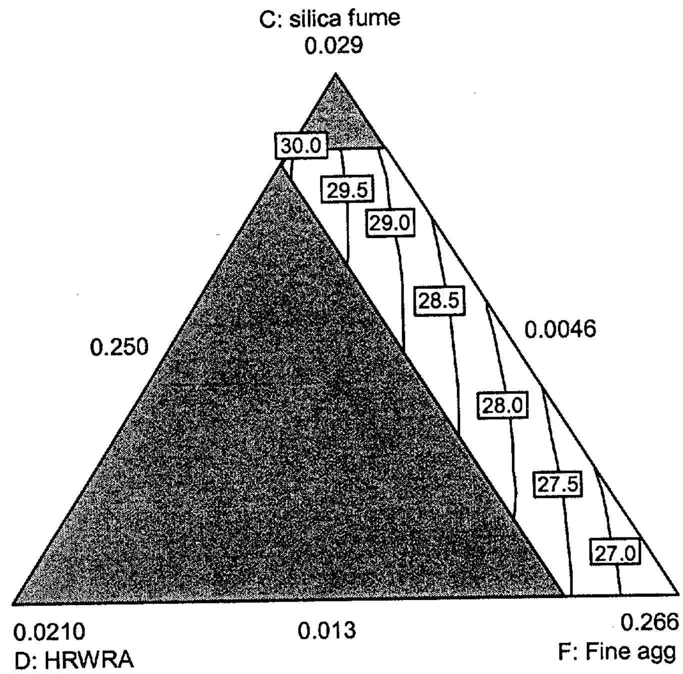


Figure A-13. Mixture experiment: contour plot of 1-day strength in silica fume, HRWRA, and fine aggregate

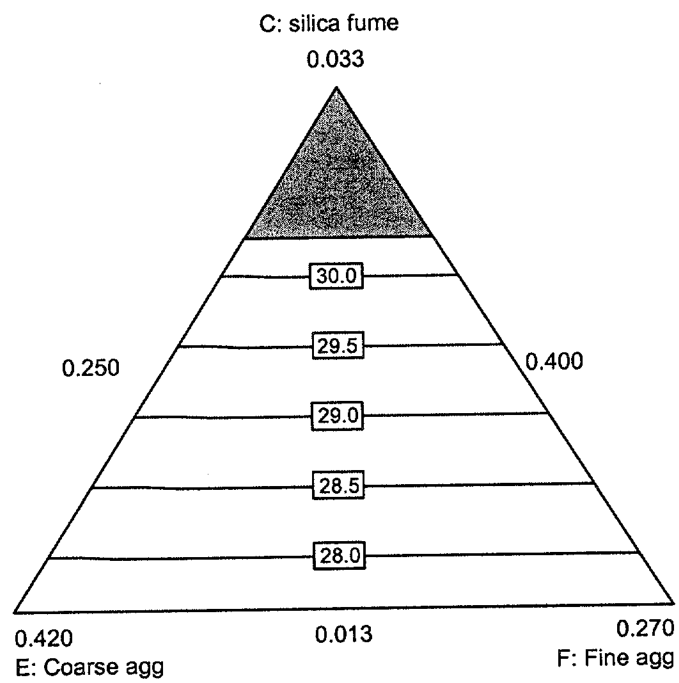


Figure A-14. Mixture experiment: contour plot of 1-day strength in silica fume, coarse aggregate, and fine aggregate

A.2.3 28-Day Strength

Table A-15. Mixture experiment: sequential model sum of squares for 28-day strength

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	106213.0	1	106213.0	–	–
Linear	257.52	5	51.50	5.46	0.0011
Quadratic	135.19	15	9.01	0.92	0.5665
Special cubic (aliased)	55.45	7	7.92	0.69	0.6826
Cubic (aliased)	0.00	0	–	–	–
Residual	92.17	8	11.52	–	–
Total	106753.3	36	2965.37	–	–

Table A-16. Mixture experiment: lack-of-fit test for 28-day strength

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Linear	190.64	22	8.67	0.75	0.7193
Quadratic	55.45	7	7.92	0.69	0.6826
Special cubic (aliased)	0.00	0	–	–	–
Cubic (aliased)	0.00	0	–	–	–
Pure error	92.17	8	11.52	–	–

Table A-17. Mixture experiment: model summary statistics for 28-day strength

Source	Std. Dev.	r^2	Adj. r^2	Pred. r^2	PRESS
Linear	3.07	0.4755	0.3894	0.2678	395.63
Quadratic	3.14	0.7268	0.3625	–1.5516	1378.72
Special cubic (aliased)	3.39	0.8294	0.2537	–	undefined
Cubic (aliased)	–	–	–	–	undefined

Table A-18. Mixture experiment: ANOVA for 28-day strength mixture model

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	257.52	5	51.50	5.46	0.0011
Linear mixture	257.52	5	51.50	5.46	0.0011
Residual	282.81	30	9.43	–	–
Lack of fit	190.64	22	8.67	0.75	0.7193
Pure error	92.17	8	11.52	–	–
Corrected total	540.33	35	–	–	–

Table A-19. Mixture experiment: estimated coefficients for 28-day strength mixture model

Component	Coeff. Estimate	DF	Std. Error	95% CI Low	95% CI High
Water	48.60	1	1.88	44.77	52.43
Cement	54.30	1	2.47	49.25	59.35
Silica fume	50.36	1	3.33	43.56	57.15
HRWRA	134.13	1	18.55	96.24	172.01
Coarse aggregate	52.14	1	1.64	48.79	55.50
Fine aggregate	54.21	1	1.72	50.70	57.73

Table A-20. Mixture experiment: adjusted effects for 28-day strength mixture model

Component	Adjusted Effect	DF	Std. Error	Approx. t for H_o Effect = 0	Prob > t
Water	-12.04	1	2.40	-5.01	< 0.0001
Cement	-6.41	1	2.31	-2.78	0.0093
Silica fume	-6.05	1	1.93	-3.13	0.0039
HRWRA	5.43	1	1.27	4.28	0.0002
Coarse aggregate	-16.17	1	3.84	-4.22	0.0002
Fine aggregate	-13.69	1	4.08	-3.35	0.0022

Model equation in terms of pseudocomponents:

28-Day Strength = 48.60*A + 54.30*B + 50.36*C + 134.13*D + 52.14*E + 54.21*F

Model equation in terms of real components:

28-Day Strength = –45.22*water + 89.15*cement – 3.809*silica fume + 1972*HRWRA + 38.36*Coarse agg + 87.19*Fine agg

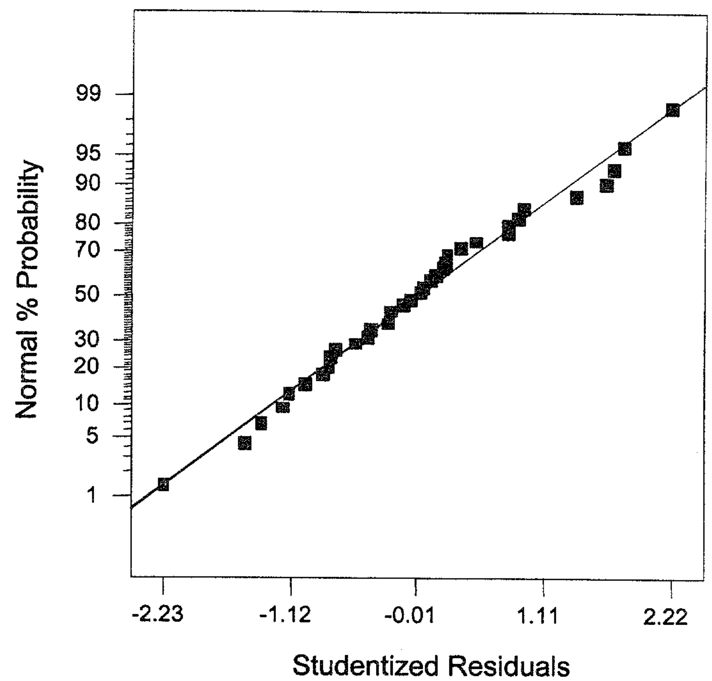


Figure A-15. Mixture experiment: normal probability plot for 28-day strength

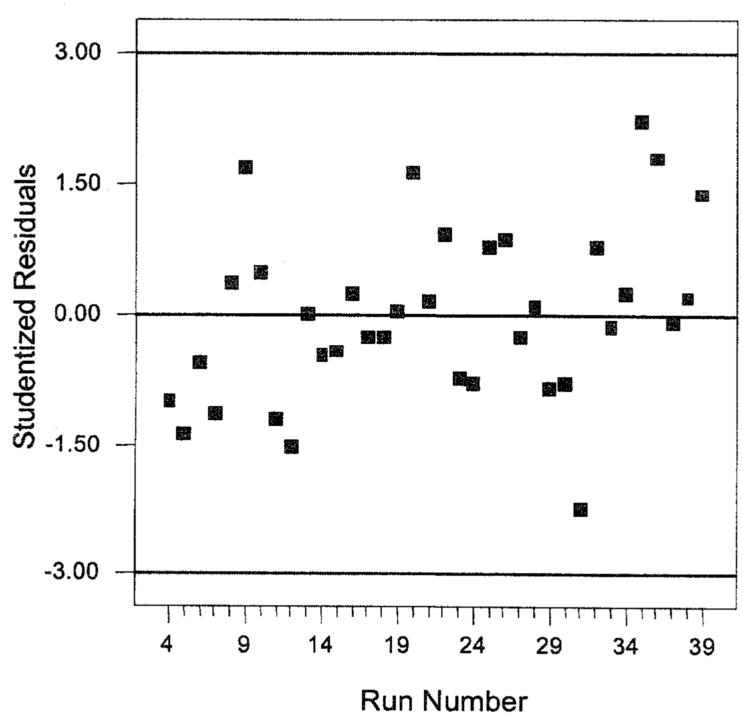


Figure A-16. Mixture experiment: residuals vs. run for 28-day strength

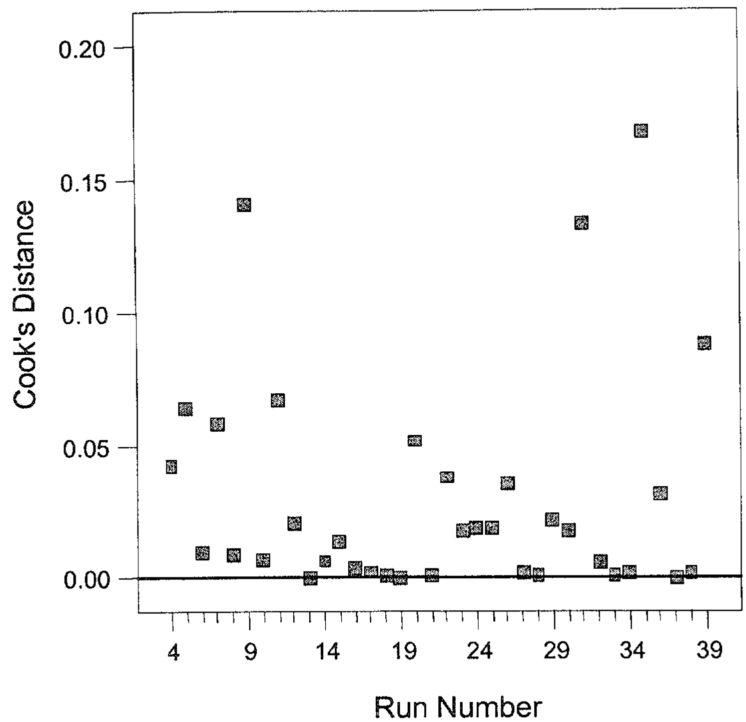


Figure A-17. Mixture experiment: Cook's distance vs. run for 28-day strength

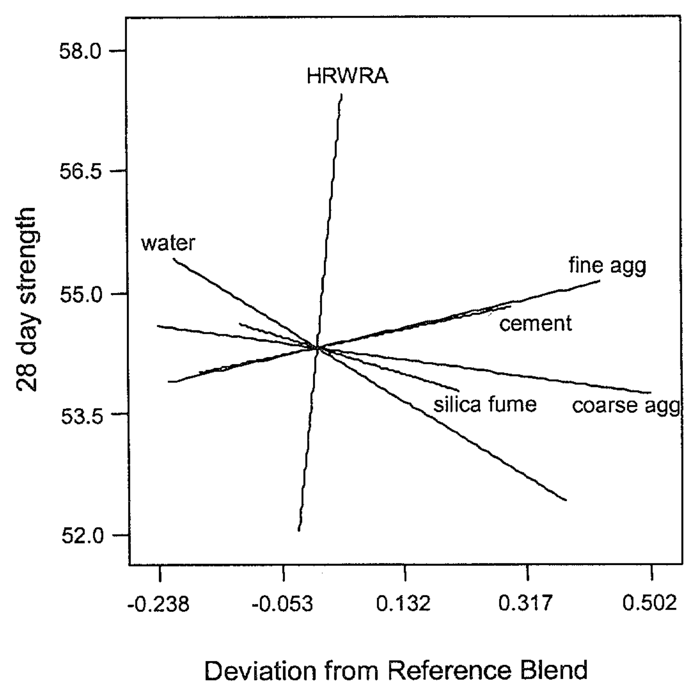


Figure A-18. Mixture experiment: trace plot for 28-day strength

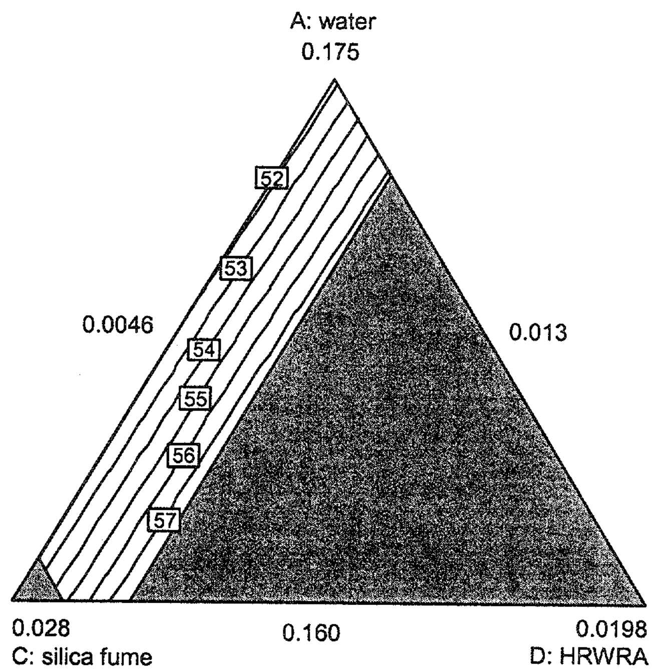


Figure A-19. Mixture experiment: contour plot of 28-day strength in water, silica fume, and HRWRA

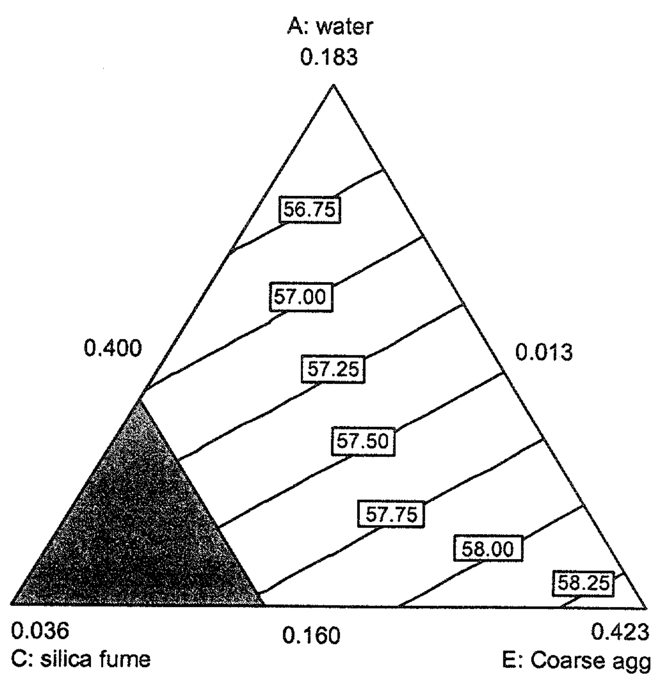


Figure A-20. Mixture experiment: contour plot of 28-day strength in water, silica fume, and coarse aggregate

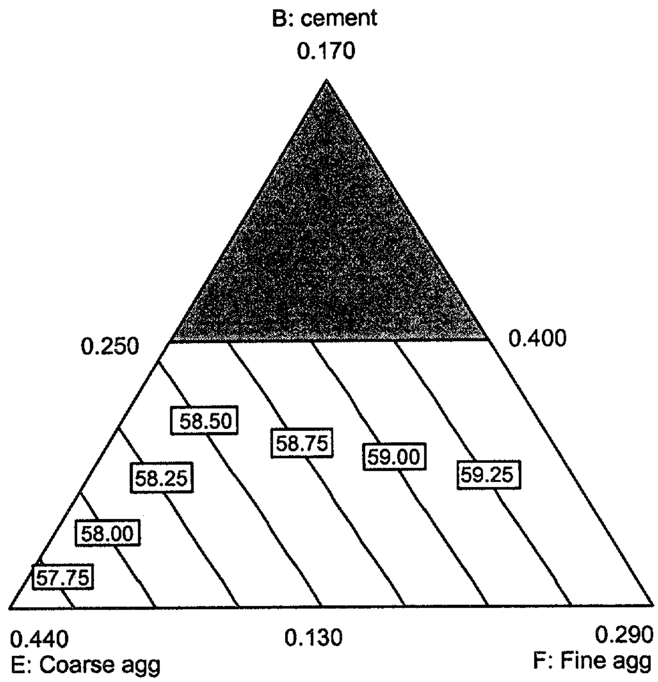


Figure A-21. Mixture experiment: contour plot of 28-day strength in cement, coarse aggregate, and fine aggregate

A.2.4 RCT Charge Passed

Table A-21. Mixture experiment: sequential model sum of squares for RCT charge passed

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	1441.26	1	1441.26	–	–
Linear	6.75	5	1.35	57.33	< 0.0001
Quadratic	0.38	15	0.03	1.17	0.3846
Special cubic (aliased)	0.11	7	0.02	0.57	0.7607
Cubic (aliased)	0.00	0	–	–	–
Residual	0.22	8	0.03	–	–
Total	1448.72	36	40.24	–	–

Table A-22. Mixture experiment: lack-of-fit test for RCT charge passed

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Linear	0.490	22	0.022	0.82	0.6666
Quadratic	0.109	7	0.016	0.57	0.7607
Special cubic (aliased)	0.000	0	–	–	–
Cubic (aliased)	0.000	0	–	–	–
Pure error	0.217	8	0.027	–	–

Table A-23. Mixture experiment: model summary statistics for RCT charge passed

Source	Std. Dev.	r^2	Adj. r^2	Pred. r^2	PRESS
Linear	0.15	0.9053	0.8895	0.8647	1.01
Quadratic	0.15	0.9563	0.8980	0.8044	1.46
Special cubic (aliased)	0.16	0.9709	0.8726	–	undefined
Cubic (aliased)	–	–	–	–	undefined

Table A-24. Mixture experiment: ANOVA for RCT charge passed mixture model

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	6.75	5	1.35	57.33	< 0.0001
Linear mixture	6.75	5	1.35	57.33	< 0.0001
Residual	0.71	30	0.024	–	–
Lack of fit	0.49	22	0.022	0.82	0.6666
Pure error	0.22	8	0.027	–	–
Corrected total	7.46	35	–	–	–

Table A-25. Mixture experiment: estimated coefficients for RCT charge passed mixture model

Component	Coeff. Estimate	DF	Std. Error	95% CI Low	95% CI High
Water	7.2	1	0.094	7.01	7.39
Cement	6.34	1	0.12	6.09	6.60
Silica fume	4.10	1	0.17	3.76	4.44
HRWRA	5.32	1	0.93	3.43	7.22
Coarse aggregate	6.62	1	0.082	6.46	6.79
Fine aggregate	6.45	1	0.086	6.28	6.63

Table A-26. Mixture experiment: adjusted effects for RCT charge passed mixture model

Component	Adjusted Effect	DF	Std. Error	Approx. t for H_o Effect = 0	Prob > t
Water	0.84	1	0.12	7.03	< 0.0001
Cement	0.19	1	0.12	1.65	0.1087
Silica fume	-0.76	1	0.097	-7.83	< 0.0001
HRWRA	-0.054	1	0.063	-0.85	0.3999
Coarse aggregate	0.74	1	0.19	3.86	0.0006
Fine aggregate	0.53	1	0.20	2.62	0.0138

Model equation in terms of pseudocomponents:

ln(RCT charge passed) = 7.20*A + 6.34*B + 4.10*C + 5.32*D + 6.62*E + 6.45*F

Model equation in terms of real components:

ln(RCT charge passed) = 20.82*water + 0.629*cement - 52.33*silica fume – 23.41*HRWRA + 7.235*Coarse agg + 3.190*Fine agg

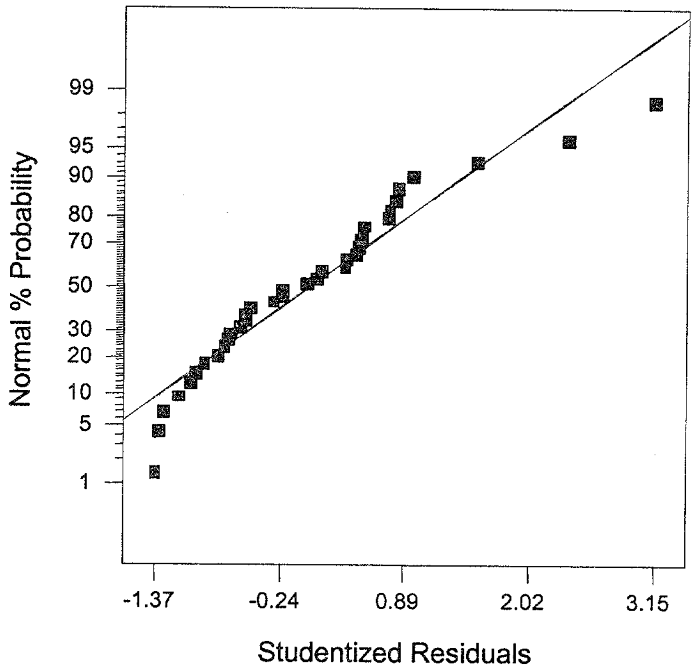


Figure A-22. Mixture experiment: normal probability plot for RCT charge passed (no transform)

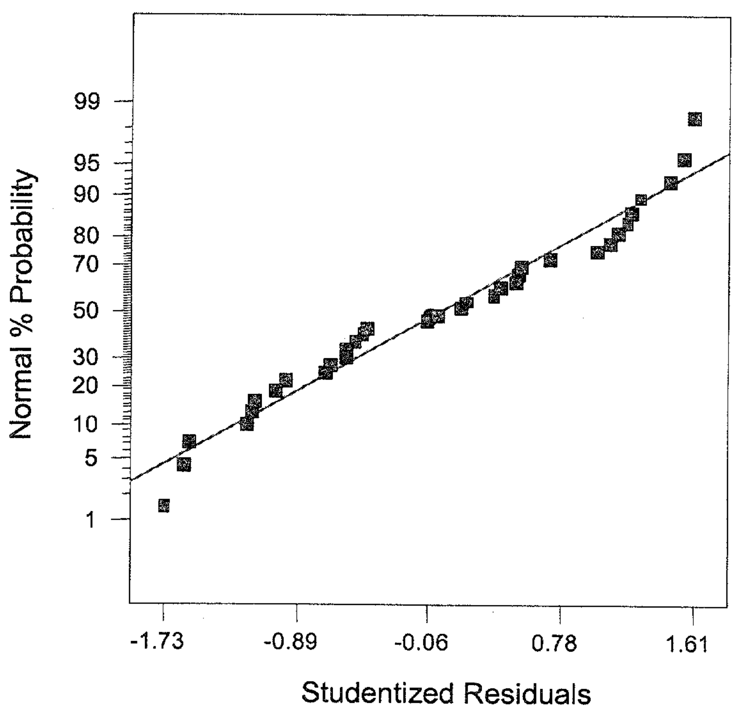


Figure A-23. Mixture experiment: normal probability plot for RCT charge passed (natural log transform)

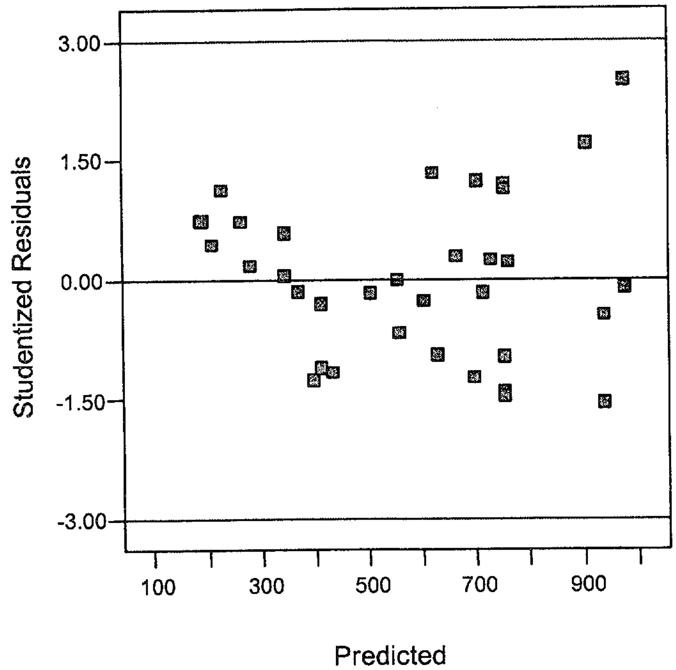


Figure A-24. Mixture experiment: residuals vs. predicted for RCT charge passed (no transform)

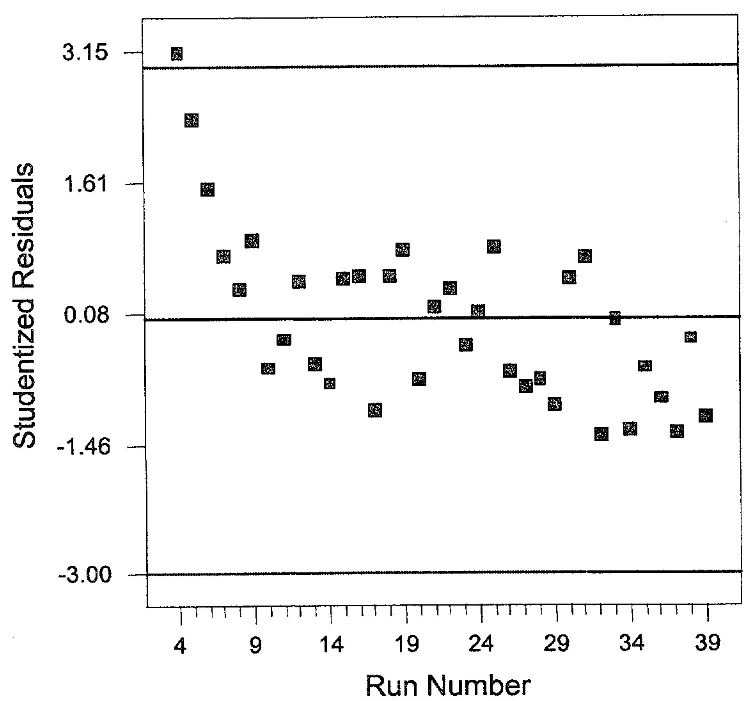


Figure A-25. Mixture experiment: residuals vs. run for RCT charge passed (no transform)

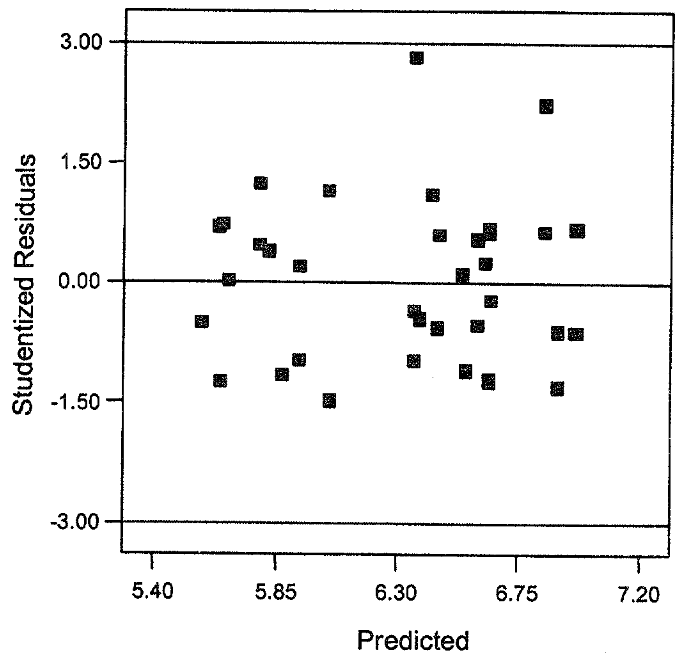


Figure A-26. Mixture experiment: residuals vs. predicted for RCT charge passed (natural log transform)

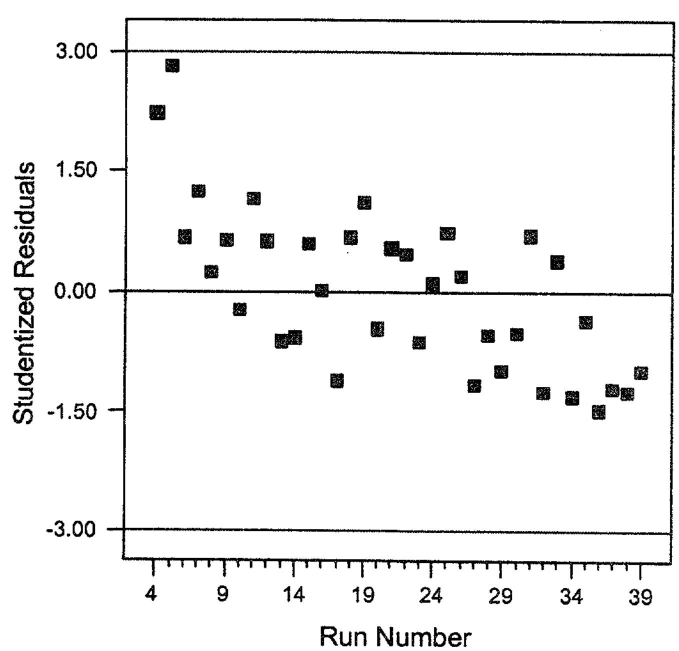


Figure A-27. Mixture experiment: residuals vs. run for RCT charge passed (natural log transform)

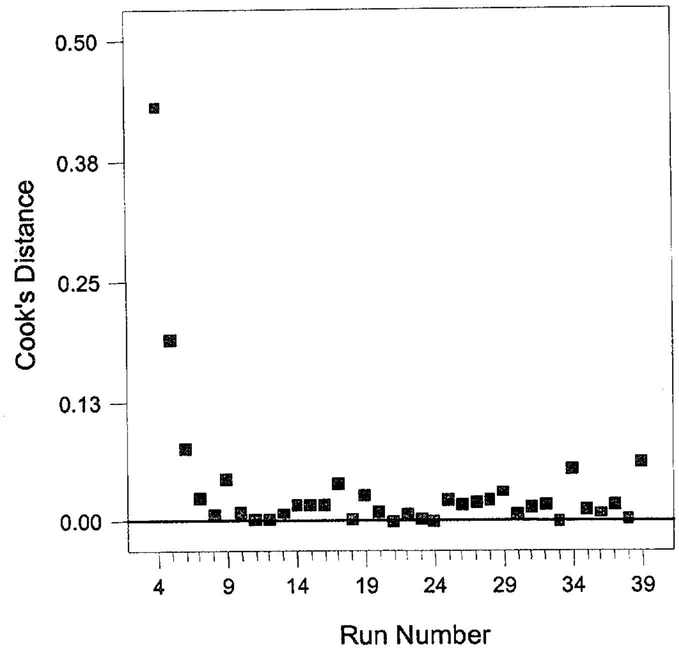


Figure A-28. Mixture experiment: Cook's distance for RCT charge passed (natural log transform)

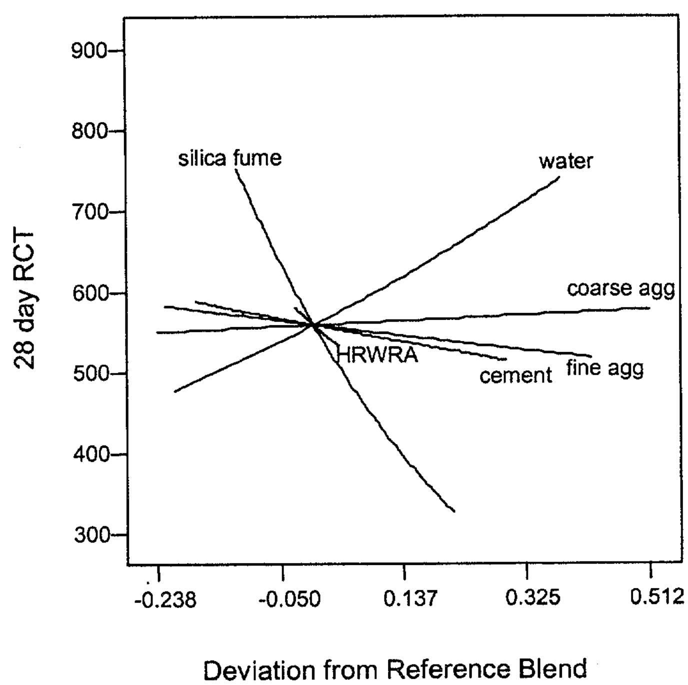


Figure A-29. Mixture experiment: trace plot for RCT charge passed (natural log transform)

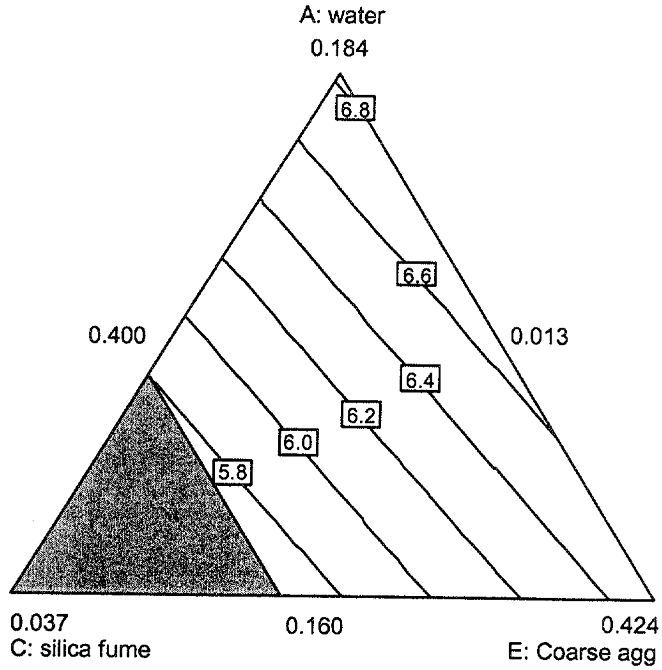


Figure A-30. Mixture experiment: contour plot of ln (RCT charge passed) in water, silica fume, and coarse aggregate

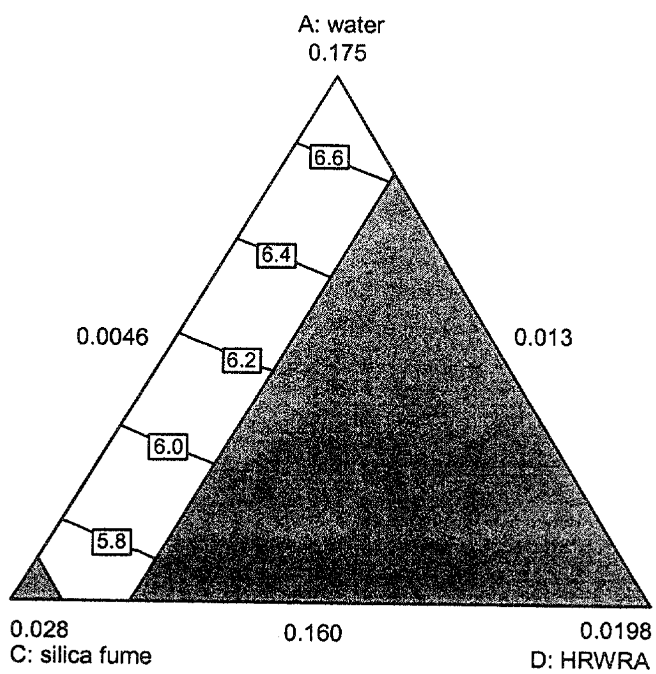


Figure A-31. Mixture experiment: contour plot of ln (RCT charge passed) in water, silica fume, and HRWRA

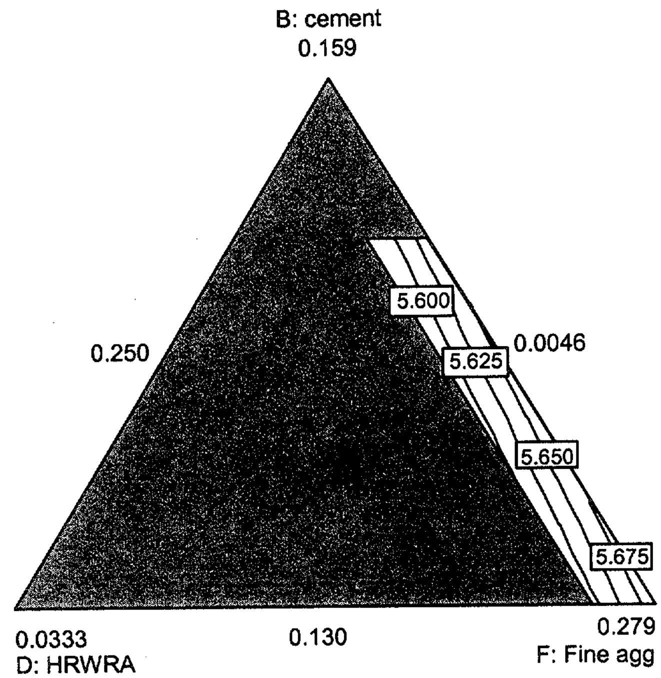


Figure A-32. Mixture experiment: contour plot of ln (RCT charge passed) in cement, HRWRA, and fine aggregate

APPENDIX B. Experiment Design and Data Analysis for Factorial Experiment

B.1 Experiment Design and Response Data

Table B-1. Factorial experiment: design by volume fraction of factors

Std Order	Run Order	Point	FactorA w/c	Factor B Fine Agg	Factor C Coarse Agg	Factor D HRWRA	Factor E Silica Fume
17	1	Center	0.39525	0.2712	0.4212	0.0060	0.0200
11	2	Fact	0.3576	0.2853	0.4071	0.0069	0.0247
7	3	Fact	0.3576	0.2853	0.4353	0.0051	0.0247
10	4	Fact	0.4329	0.2571	0.4071	0.0069	0.0247
4	5	Fact	0.4329	0.2853	0.4071	0.0051	0.0247
12	6	Fact	0.4329	0.2853	0.4071	0.0069	0.0153
2	7	Fact	0.4329	0.2571	0.4071	0.0051	0.0153
1	8	Fact	0.3576	0.2571	0.4071	0.0051	0.0247
18	9	Center	0.39525	0.2712	0.4212	0.0060	0.0200
8	10	Fact	0.4329	0.2853	0.4353	0.0051	0.0153
9	11	Fact	0.3576	0.2571	0.4071	0.0069	0.0153
6	12	Fact	0.4329	0.2571	0.4353	0.0051	0.0247
3	13	Fact	0.3576	0.2853	0.4071	0.0051	0.0153
14	14	Fact	0.4329	0.2571	0.4353	0.0069	0.0153
15	15	Fact	0.3576	0.2853	0.4353	0.0069	0.0153
13	16	Fact	0.3576	0.2571	0.4353	0.0069	0.0247
19	17	Center	0.39525	0.2712	0.4212	0.0060	0.0200
5	18	Fact	0.3576	0.2571	0.4353	0.0051	0.0153
16	19	Fact	0.4329	0.2853	0.4353	0.0069	0.0247
25	20	Axial	0.39525	0.2712	0.4494	0.0060	0.0200
21	21	Axial	0.47055	0.2712	0.4212	0.0060	0.0200
23	22	Axial	0.39525	0.2994	0.4212	0.0060	0.0200
27	23	Axial	0.39525	0.2712	0.4212	0.0078	0.0200
20	24	Axial	0.31995	0.2712	0.4212	0.0060	0.0200
31	25	Center	0.39525	0.2712	0.4212	0.0060	0.0200
26	26	Axial	0.39525	0.2712	0.4212	0.0042	0.0200
28	27	Axial	0.39525	0.2712	0.4212	0.0060	0.0106
24	28	Axial	0.39525	0.2712	0.3930	0.0060	0.0200
29	29	Axial	0.39525	0.2712	0.4212	0.0060	0.0294
22	30	Axial	0.39525	0.243	0.4212	0.0060	0.0200
30	31	Center	0.39525	0.2712	0.4212	0.0060	0.0200

Table B-2. Factorial experiment: slump and 1-day strength data

Run	Point	Slump (mm)		1-Day Strength (MPa)		
1	Center	76	70	16.6	16.0	16.2
2	Fact	44	44	22.2	22.5	23.0
3	Fact	13	13	22.5	17.9	22.0
4	Fact	102	102	15.8	16.7	16.8
5	Fact	57	57	16.4	16.7	16.1
6	Fact	140	146	13.4	14.2	13.2
7	Fact	70	64	13.9	11.1	13.7
8	Fact	13	13	17.7	22.8	20.5
9	Center	89	83	17.9	18.6	18.7
10	Fact	102	102	15.2	15.2	15.2
11	Fact	140	140	20.9	20.7	20.4
12	Fact	32	32	13.8	18.8	18.9
13	Fact	13	13	24.5	23.3	24.7
14	Fact	76	76	17.3	17.2	17.2
15	Fact	13	13	22.7	19.5	21.8
16	Fact	13	13	20.8	20.6	21.4
17	Center	51	64	19.4	18.9	18.1
18	Fact	32	25	21.4	22.2	22.1
19	Fact	38	32	16.0	16.1	16.3
20	Axial	38	38	18.7	19.3	18.9
21	Axial	121	114	14.5	14.9	14.0
22	Axial	70	64	18.0	17.8	17.5
23	Axial	64	64	19.3	20.0	20.4
24	Axial	19	13	26.0	25.4	27.7
25	Center	83	76	20.2	17.3	19.6
26	Axial	64	64	18.9	19.5	18.9
27	Axial	152	152	16.4	17.0	16.9
28	Axial	95	95	20.1	20.8	19.7
29	Axial	38	32	17.2	20.1	18.0
30	Axial	102	102	17.7	17.0	17.7
31	Center	76	76	16.8	19.6	18.8

Table B-3. Factorial experiment: 28-day strength and RCT charge passed data

Run	Point	28-Day Strength (MPa)				RCT Charge Passed (coulombs)		
1	Center	54.0	63.0	–	–	263	296	300
2	Fact	59.4	60.2	–	–	186	472	268
3	Fact	53.5	52.8	51.7	–	151	151	178
4	Fact	62.7	60.8	55.1	62.9	280	329	279
5	Fact	52.6	56.6	55.8	–	273	236	262
6	Fact	60.4	52.1	60.6	61.3	553	585	485
7	Fact	50.1	49.4	51.5	–	468	550	490
8	Fact	51.0	56.3	47.2	55.2	253	240	208
9	Center	63.5	62.5	–	–	247	315	305
10	Fact	53.8	54.2	56.3	–	460	437	439
11	Fact	61.6	64.5	60.8	–	415	427	393
12	Fact	56.5	55.3	56.8	–	258	258	240
13	Fact	58.1	50.2	54.4	–	343	362	317
14	Fact	52.3	46.6	52.1	–	596	527	481
15	Fact	60.3	58.7	58.6	–	218	288	330
16	Fact	60.2	58.5	62.9	–	208	194	216
17	Center	59.9	54.5	55.5	–	299	327	318
18	Fact	58.4	60.1	56.3	–	360	364	340
19	Fact	65.0	59.9	63.9	–	242	243	206
20	Axial	56.7	57.0	62.1	–	168	242	224
21	Axial	53.9	51.1	56.7	–	463	461	449
22	Axial	60.7	62.9	63.6	–	319	305	257
23	Axial	68.4	66.8	67.1	–	272	280	251
24	Axial	62.1	59.4	54.0	–	190	184	192
25	Center	58.2	55.8	56.8	–	239	246	287
26	Axial	52.9	48.2	51.6	–	258	281	280
27	Axial	51.3	55.2	56.8	–	704	766	644
28	Axial	50.0	55.2	54.8	–	268	302	351
29	Axial	55.5	53.8	56.2	–	163	170	153
30	Axial	50.4	49.0	51.6	–	340	304	351
31	Center	55.8	53.3	56.5	–	262	294	274

B.2 Data Analysis and Model Fitting

B.2.1 Slump

Table B-4. Factorial experiment: sequential model sum of squares for slump

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	130296.6	1	130296.6	–	–
Linear	31972.38	5	6394.48	9.10	< 0.0001
2FI	10539.29	10	1053.93	2.25	0.0755
Quadratic	2598.70	5	519.74	1.18	0.3856
Cubic (aliased)	2316.86	5	463.37	1.10	0.4593
Residual	2104.40	5	420.88	–	–
Total	179828.3	31	5800.91	–	–

Table B-5. Factorial experiment: lack-of-fit test for slump

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Linear	17103.61	21	814.46	7.15	0.0345
2FI	6564.32	11	596.76	5.24	0.0618
Quadratic	3965.62	6	660.94	5.80	0.0553
Cubic (aliased)	1648.75	1	1648.75	14.47	0.0190
Pure error	455.64	4	113.91	–	–

Table B-6. Factorial experiment: ANOVA for slump model

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	40109.97	7	5730.00	13.99	< 0.0001
A	12138.75	1	12138.75	29.63	< 0.0001
B	606.52	1	606.52	1.48	0.2360
C	6048.38	1	6048.38	14.77	0.0008
D	2426.07	1	2426.07	5.92	0.0231
E	10752.67	1	10752.67	26.25	< 0.0001
AB	1837.19	1	1837.19	4.48	0.0452
CD	6300.39	1	6300.39	15.38	0.0007
Residual	9421.67	23	409.64	–	–
Lack of fit	8966.03	19	471.90	4.14	0.0887
Pure error	455.64	4	113.91	–	–
Cor total	49531.64	30	–	–	–

Table B-7. Factorial experiment: summary statistics for slump model

Std. Dev.	20.24	R-Squared	0.8098
Mean	64.83	Adj R-Squared	0.7519
C.V.	31.22	Pred R-Squared	0.6275
PRESS	18452.19	Adeq Precision	15.6200

Table B-8. Factorial experiment: coefficient estimates for slump model

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High
Intercept	64.83	1	3.64	57.31	72.35
A (w/c)	22.49	1	4.13	13.94	31.04
B (fine agg)	-5.03	1	4.13	-13.57	3.52
C (coarse agg)	-15.87	1	4.13	-24.42	-7.33
D (HRWRA)	10.05	1	4.13	1.51	18.60
E (silica fume)	-21.17	1	4.13	-29.71	-12.62
AB	10.72	1	5.06	0.25	21.18
CD	-19.84	1	5.06	-30.31	-9.38

Model equation for slump in terms of coded factors:

$$\text{Slump} = 64.83 + 22.49*A - 5.03*B - 15.87*C + 10.05*D - 21.17*E + 10.72*A*B - 19.84*C*D$$

Model equation for slump in terms of actual factors:

$$\text{Slump} = -1365.5 - 4876.9*\text{w/c} - 8334.7*\text{fine agg} + 8256.5*\text{coarse agg} + 6.6982 \times 10^{5}*\text{HRWRA} - 4503.6*\text{silica fume} + 20185*\text{w/c}*\text{fine agg} - 1.564 \times 10^{6}*\text{coarse agg}*\text{HRWRA}$$

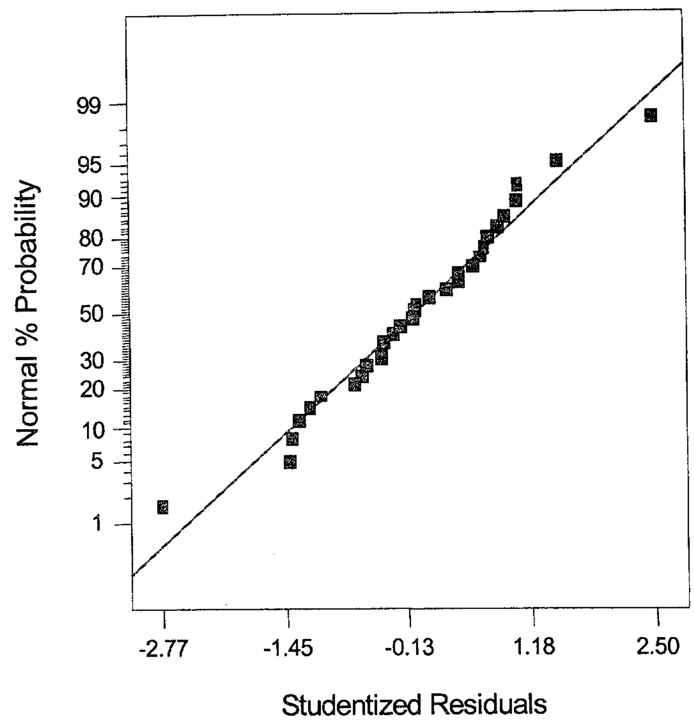


Figure B-1. Factorial experiment: normal probability plot for slump

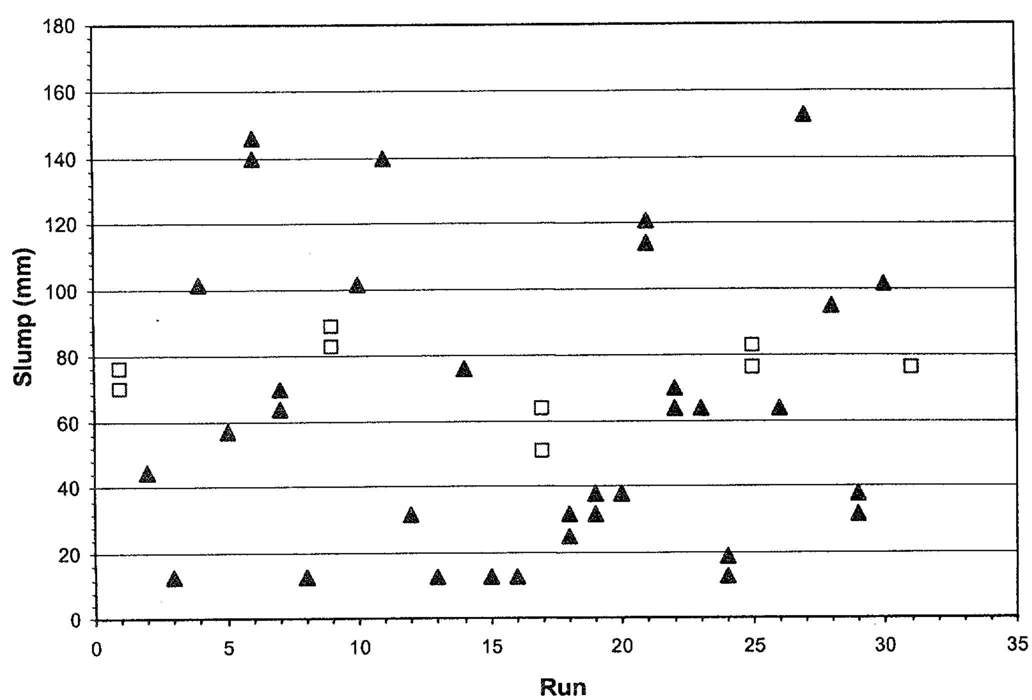


Figure B-2. Factorial experiment: raw data plot for slump (hollow squares indicate control runs)

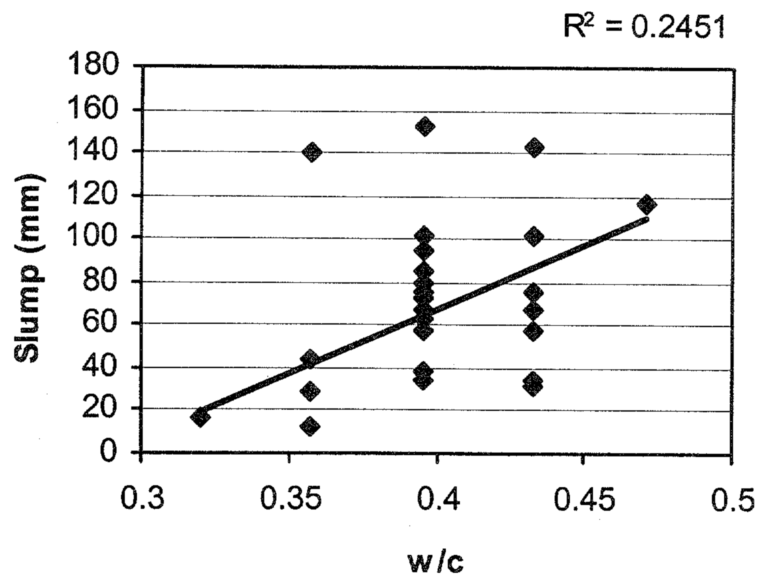


Figure B-3. Factorial experiment: scatterplot of slump vs. w/c

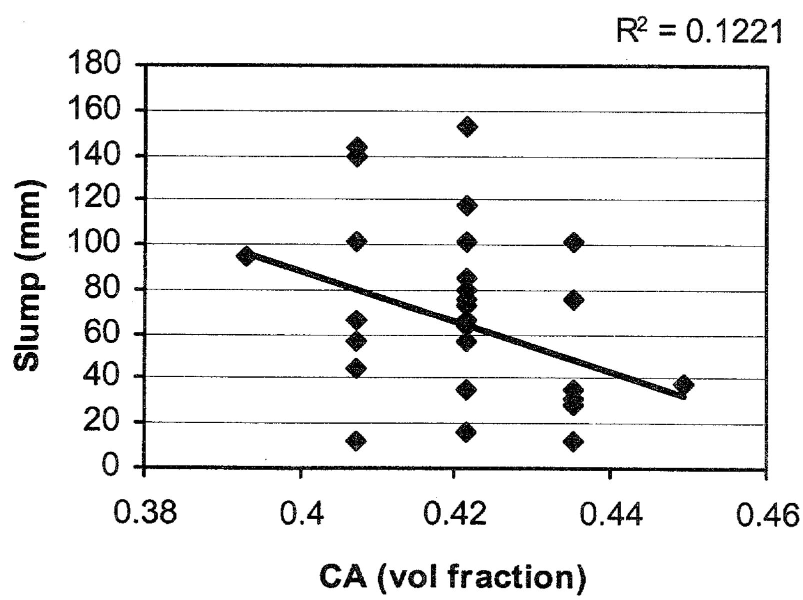


Figure B-4. Factorial experiment: scatterplot of slump vs. coarse aggregate

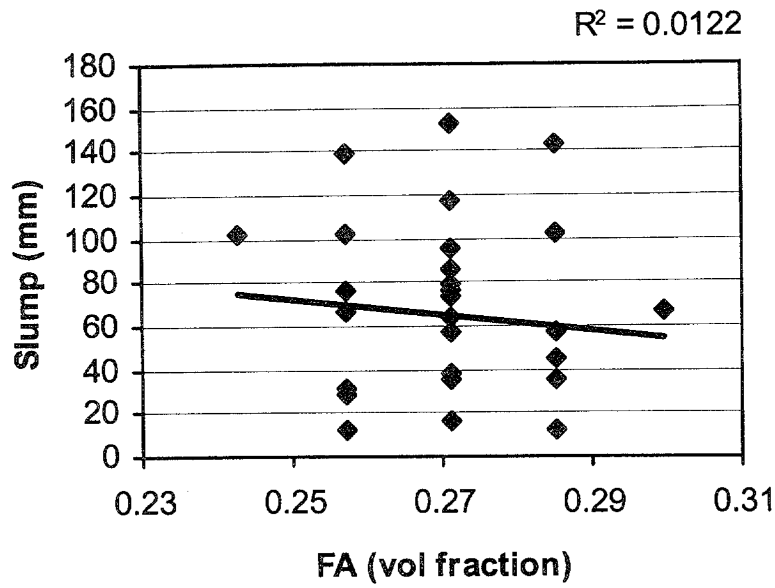


Figure B-5. Factorial experiment: scatterplot of slump vs. fine aggregate

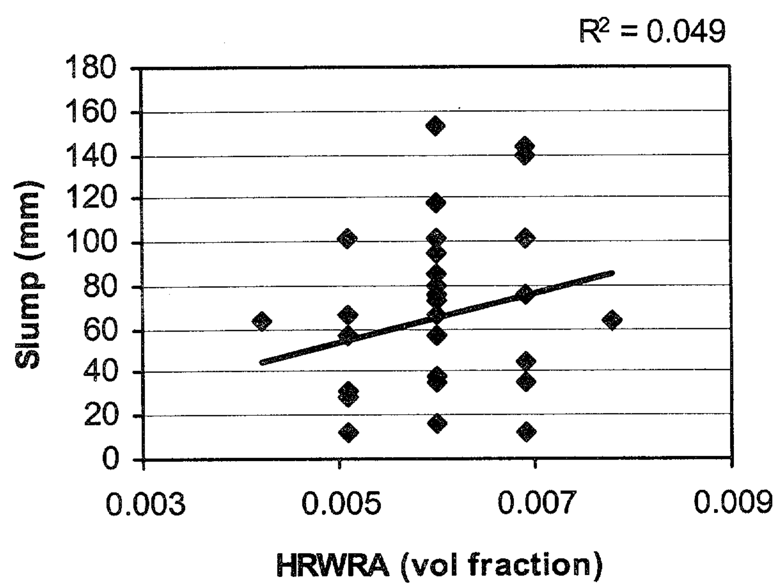


Figure B-6. Factorial experiment: scatterplot of slump vs. HRWRA

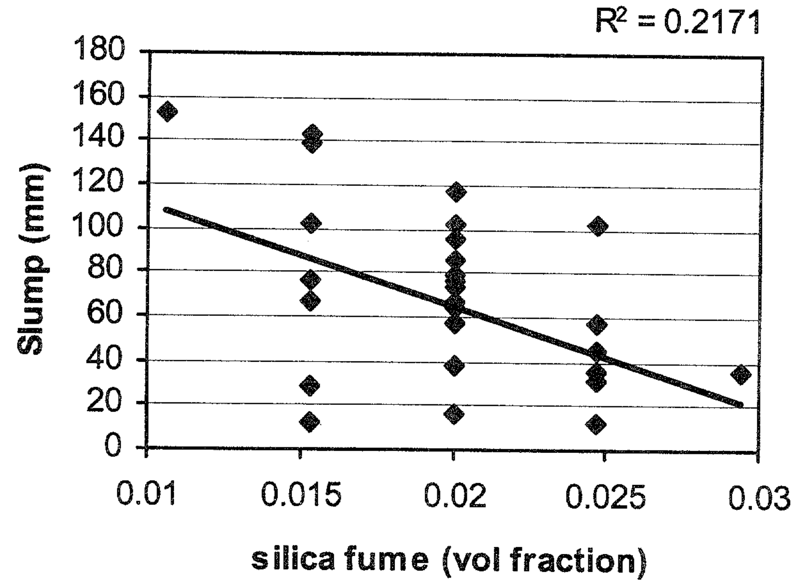


Figure B-7. Factorial experiment: scatterplot of slump vs. silica fume

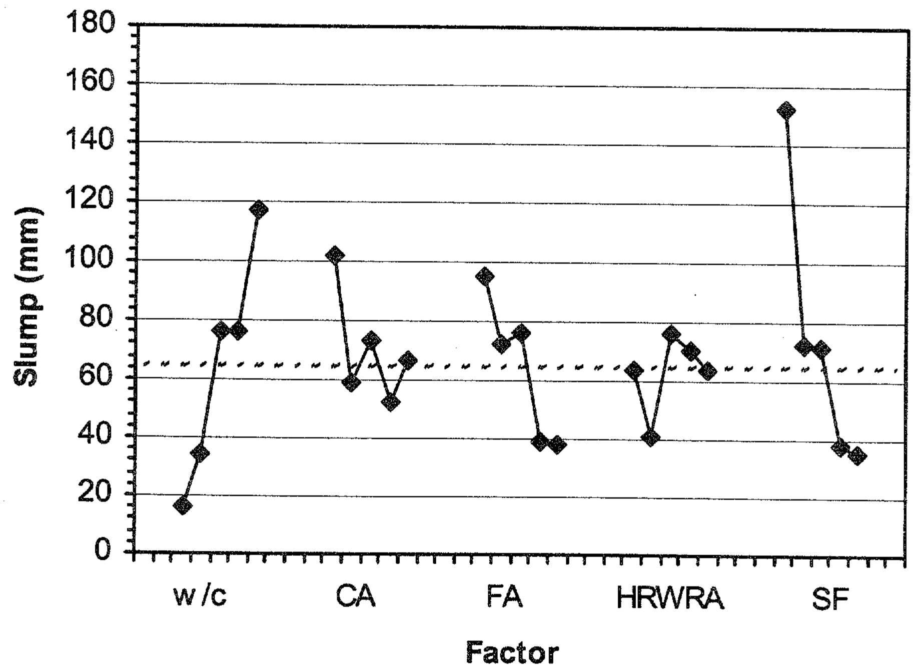


Figure B-8. Factorial experiment: means plots for slump

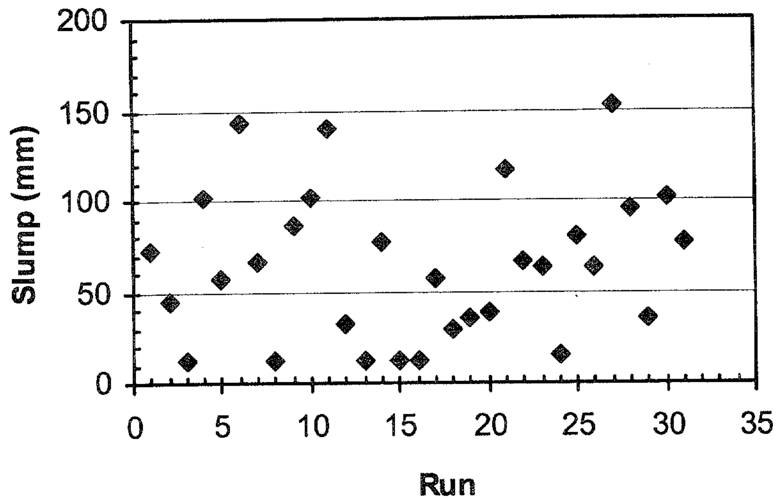


Figure B-9. Factorial experiment: slump vs. run sequence

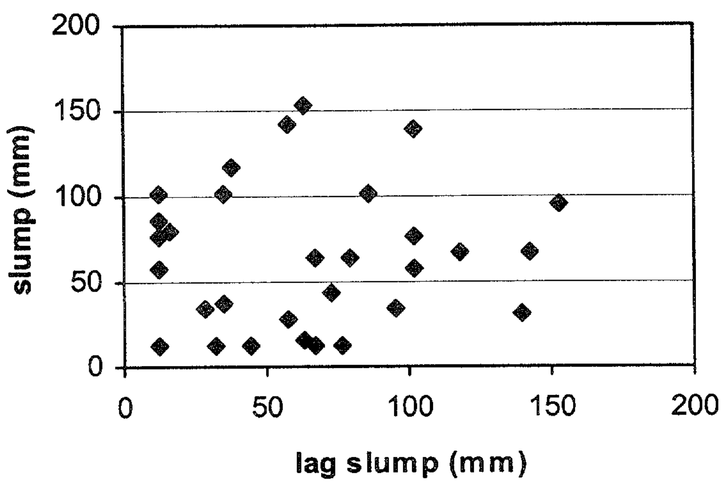


Figure B-10. Factorial experiment: lag plot for slump

B.2.2 1-Day Strength

Table B-9. Factorial experiment: sequential model sum of squares for 1-day strength

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	10780.54	1	10780.54	–	–
Linear	215.97	5	43.19	22.15	< 0.0001
2FI	27.35	10	2.73	1.92	0.1236
Quadratic	13.60	5	2.72	3.48	0.0441
Cubic (aliased)	1.86	5	0.37	0.31	0.8865
Residual	5.95	5	1.19	–	–
Total	11045.26	31	356.30	–	–

Table B-10. Factorial experiment: lack-of-fit test for 1-day strength

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Linear	43.98	21	2.09	1.75	0.3129
2FI	16.63	11	1.51	1.27	0.4444
Quadratic	3.03	6	0.51	0.42	0.8339
Cubic (aliased)	1.18	1	1.18	0.98	0.3772
Pure error	4.78	4	1.19	–	–

Table B-11. Factorial experiment: ANOVA for 1-day strength model

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	240.87	8	30.11	27.76	< 0.0001
A	213.26	1	213.26	196.66	< 0.0001
B	0.48	1	0.48	0.45	0.5113
C	0.043	1	0.043	0.040	0.8433
E	2.06	1	2.06	1.90	0.1819
A^2	6.20	1	6.20	5.72	0.0257
AC	5.15	1	5.15	4.75	0.0404
AE	7.16	1	7.16	6.60	0.0175
BC	6.51	1	6.51	6.00	0.0227
Residual	23.86	22	1.08	–	–
Lack of fit	19.08	18	1.06	0.89	0.6248
Pure error	4.78	4	1.19	–	–
Cor total	264.72	30	–	–	–

Table B-12. Factorial experiment: summary statistics for 1-day strength model

Std. Dev.	1.04	R-Squared	0.9099
Mean	18.65	Adj R-Squared	0.8771
C.V.	5.58	Pred R-Squared	0.8294
PRESS	45.16	Adeq Precision	22.583

Table B-13. Factorial experiment: coefficient estimates for 1-day strength model

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High
Intercept	18.29	1	0.24	17.80	18.79
A (w/c)	-2.98	1	0.21	-3.42	-2.54
B (fine agg)	0.14	1	0.21	-0.30	0.58
C (coarse agg)	0.043	1	0.21	-0.40	0.48
E (silica fume)	0.29	1	0.21	-0.15	0.73
A^2	0.46	1	0.19	0.061	0.86
AC	0.57	1	0.26	0.027	1.11
AE	0.67	1	0.26	0.13	1.21
BC	-0.64	1	0.26	-1.18	-0.098

Model equation for 1-day strength in terms of coded factors:

$$\text{1-day strength} = 18.29 - 2.98*A + 0.14*B + 0.043*C + 0.29*E + 0.46*A^2 + 0.57*A*C + 0.67*A*E - 0.64*B*C$$

Model equation for 1-day strength in terms of actual factors:

$$\text{1-day strength} = -63.8 - 860.8*\text{w/c} + 1361.3*\text{fine agg} + 450.8*\text{coarse agg} - 1431.5*\text{silica fume} + 323.9*(\text{w/c})^2 + 1068*\text{w/c}*\text{coarse agg} + 3780*\text{w/c}*\text{silica fume} - 3208*\text{fine agg}*\text{coarse agg}$$

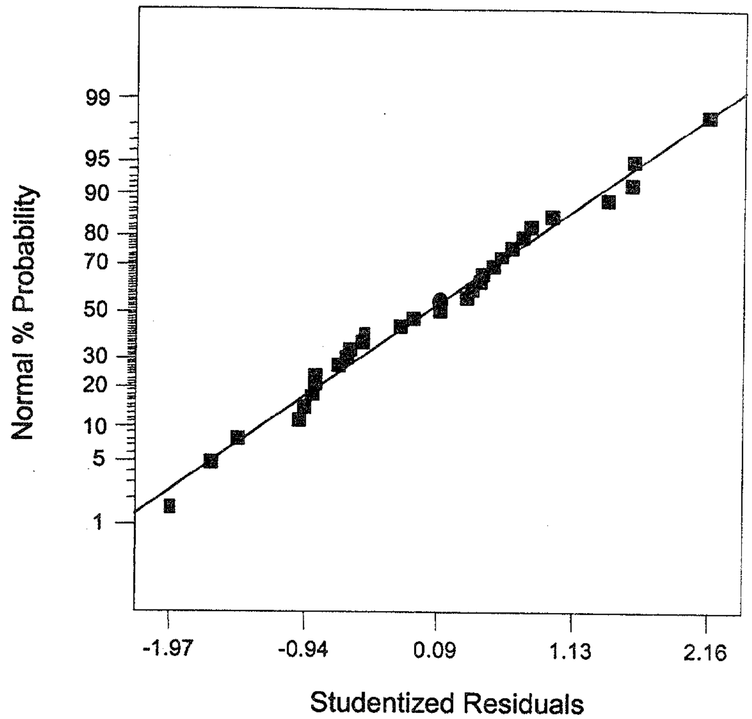


Figure B-11. Factorial experiment: normal probability plot for 1-day strength

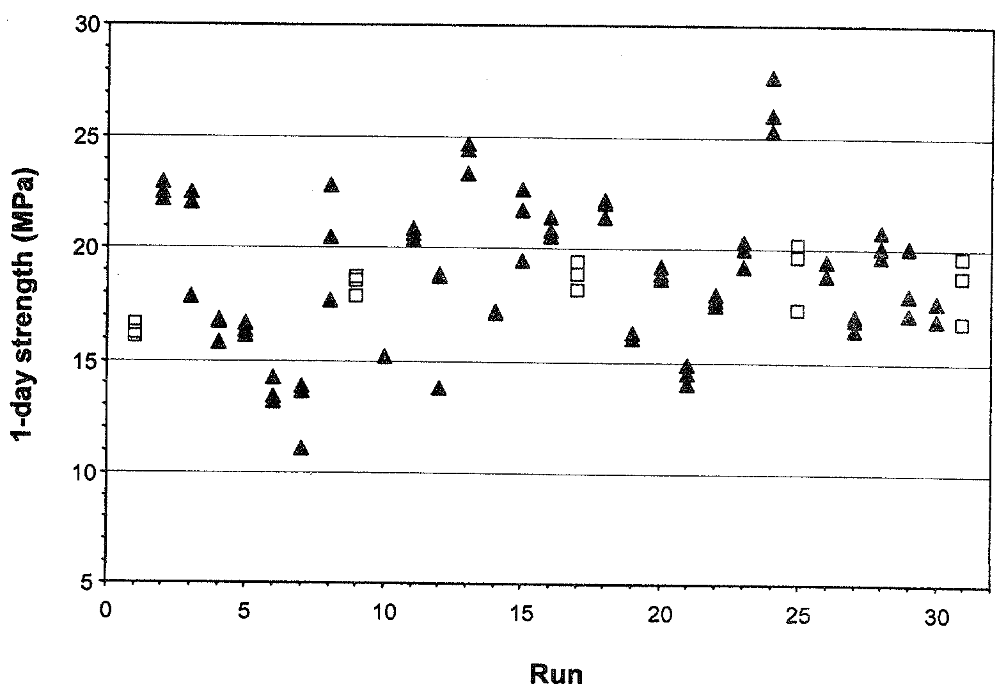


Figure B-12. Factorial experiment: raw data plot for 1-day strength (hollow squares indicate control runs)

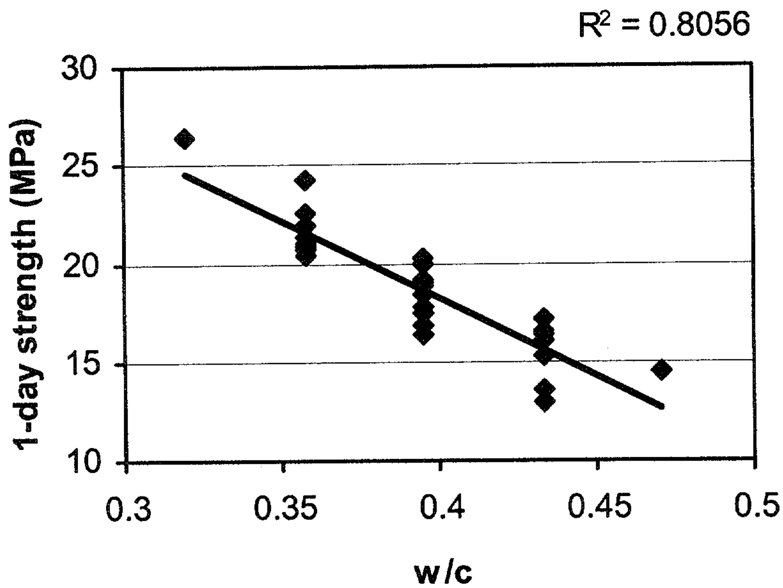


Figure B-13. Factorial experiment: scatterplot of 1-day strength vs. w/c

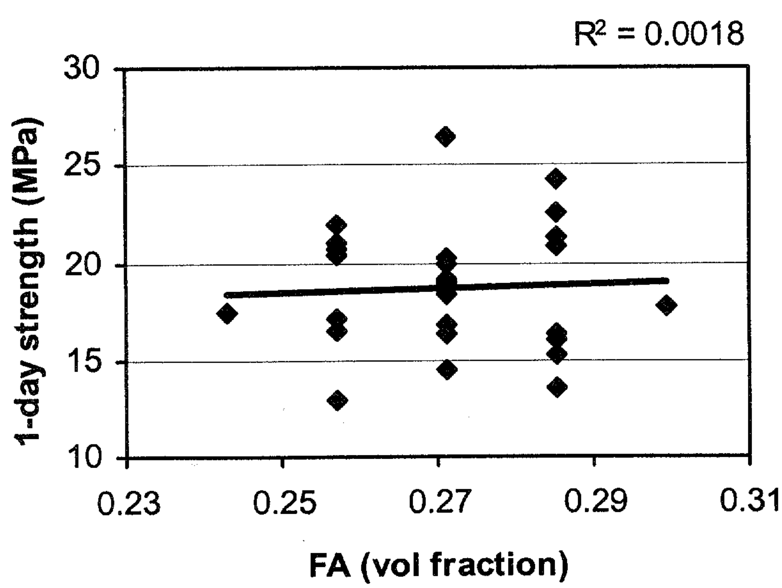


Figure B-14. Factorial experiment: scatterplot of 1-day strength vs. fine aggregate

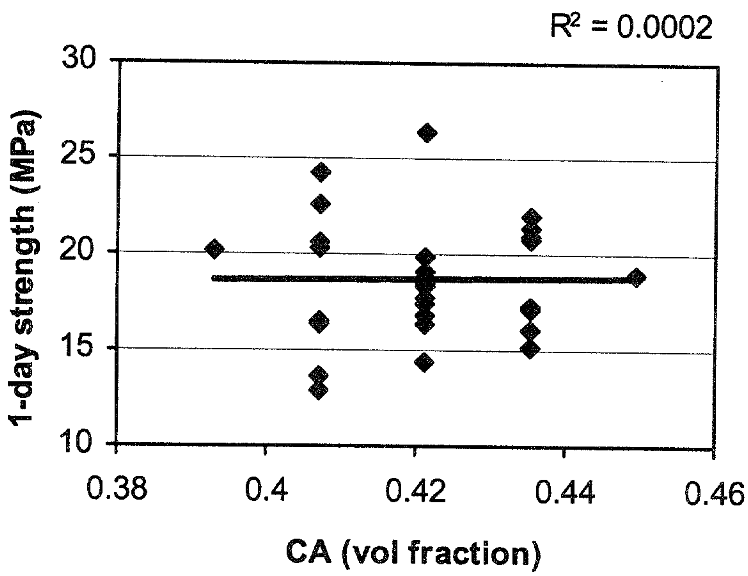


Figure B-15. Factorial experiment: scatterplot of 1-day strength vs. coarse aggregate

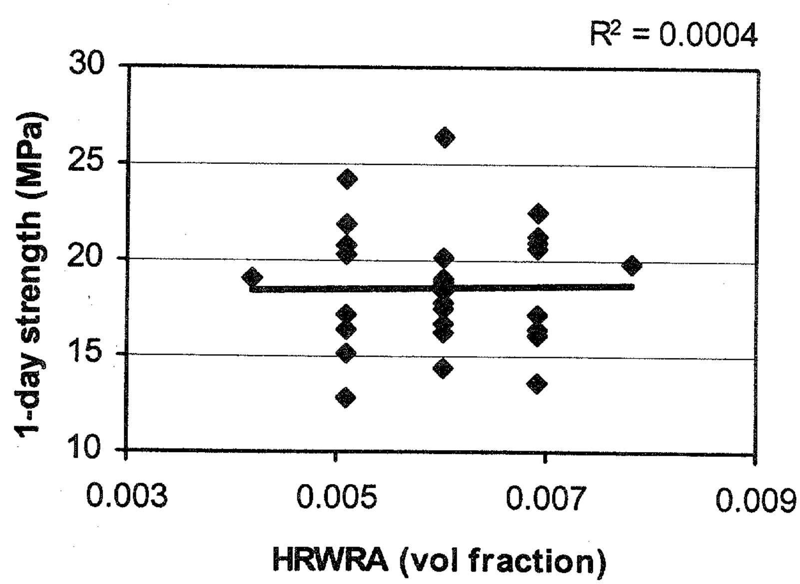


Figure B-16. Factorial experiment: scatterplot of 1-day strength vs. HRWRA

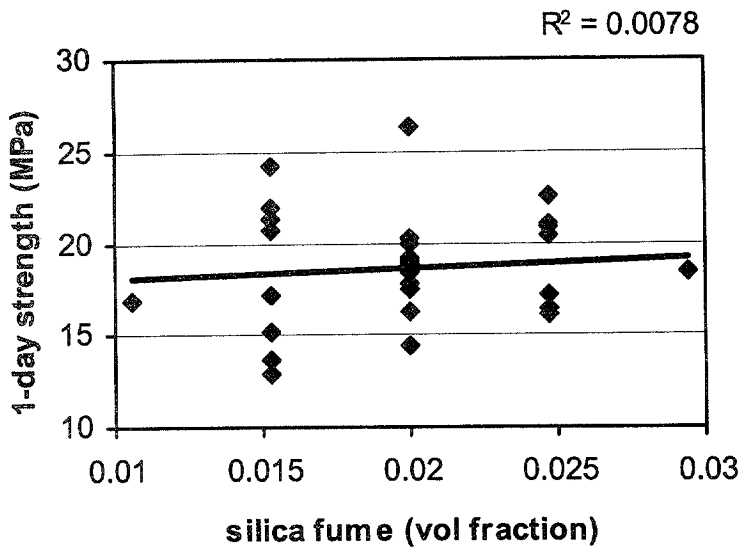


Figure B-17. Factorial experiment: scatterplot of 1-day strength vs. silica fume

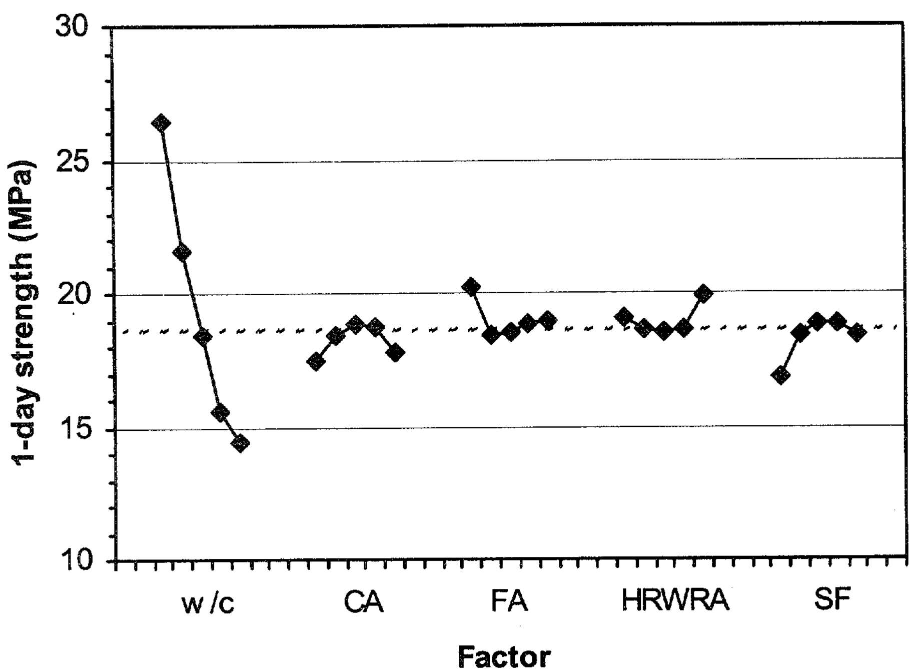


Figure B-18. Factorial experiment: means plot for 1-day strength

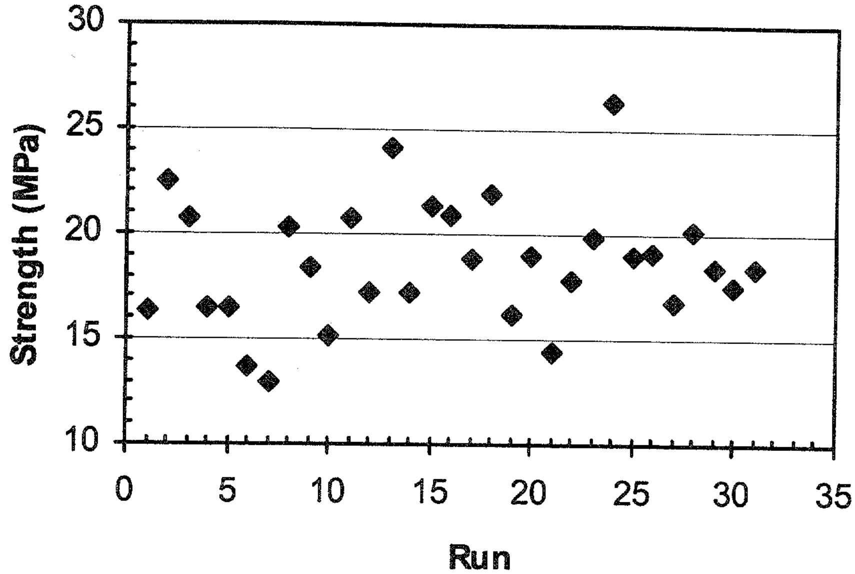


Figure B-19. Factorial experiment: 1-day strength vs. run sequence

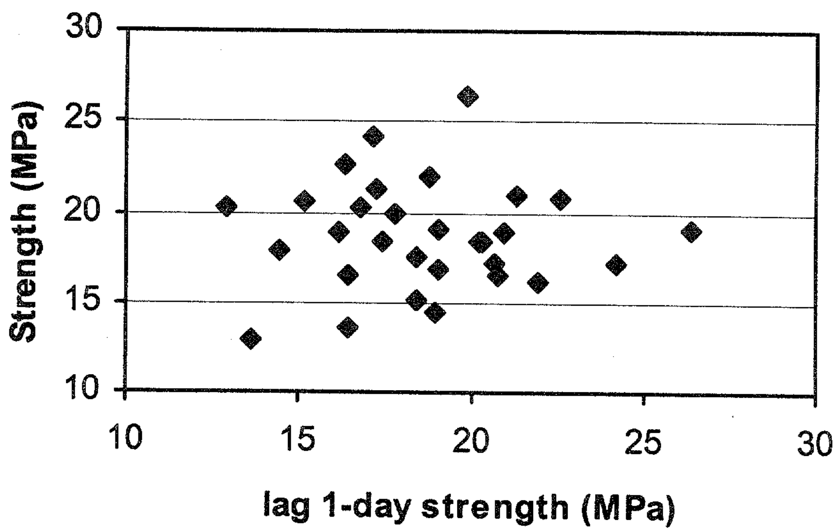


Figure B-20. Factorial experiment: lag plot for 1-day strength

B.2.3. 28-Day Strength

Table B-14. Factorial experiment: sequential model sum of squares for 28-day strength

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	100300.0	1	100300.0	–	–
Linear	292.28	5	58.46	5.71	0.0012
2FI	129.24	10	12.92	1.53	0.2208
Quadratic	27.53	5	5.51	0.56	0.7318
Cubic (aliased)	61.25	5	12.25	1.62	0.3050
Residual	37.84	5	7.57	–	–
Total	100848.1	31	3253.17	–	–

Table B-15. Factorial experiment: lack-of-fit test for 28-day strength

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Linear	219.79	21	10.47	1.16	0.4972
2FI	90.55	11	8.23	0.91	0.5942
Quadratic	63.02	6	10.50	1.16	0.4620
Cubic (aliased)	1.76	1	1.76	0.20	0.6813
Pure error	36.08	4	9.02	–	–

Table B-16. Factorial experiment: ANOVA for 28-day strength model

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	300.21	4	75.05	7.87	0.0003
A	16.57	1	16.57	1.74	0.1990
D	223.41	1	223.41	23.43	< 0.0001
E	7.47	1	7.47	0.78	0.3842
AE	52.76	1	52.76	5.53	0.0265
Residual	247.94	26	9.54	–	–
Lack of fit	211.86	22	9.63	1.07	0.5389
Pure error	36.08	4	9.02	–	–
Cor total	548.15	30	–	–	–

Table B-17. Factorial experiment: summary statistics for 28-day strength model

Std. Dev.	3.09	R-Squared	0.5477
Mean	56.88	Adj R-Squared	0.4781
C.V.	5.43	Pred R-Squared	0.3997
PRESS	329.05	Adeq Precision	9.964

Table B-18. Factorial experiment: coefficient estimates for 28-day strength model

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High
Intercept	56.88	1	0.55	55.74	58.02
A (w/c)	-0.83	1	0.63	-2.13	0.46
D (HRWRA)	3.05	1	0.63	1.76	4.35
E (silica fume)	0.56	1	0.63	-0.74	1.85
AE	1.82	1	0.77	0.23	3.40

Model equation for 28-day strength in terms of coded factors:

28-day strength = 56.88 – 0.83*A + 3.05*D + 0.56*E + 1.82*A*E

Model equation for 28-day strength in terms of actual factors:

28-day strength = 124.0 – 227.3*w/c + 3390*HRWRA – 3937.5*silica fume
+ 10262*w/c*silica fume

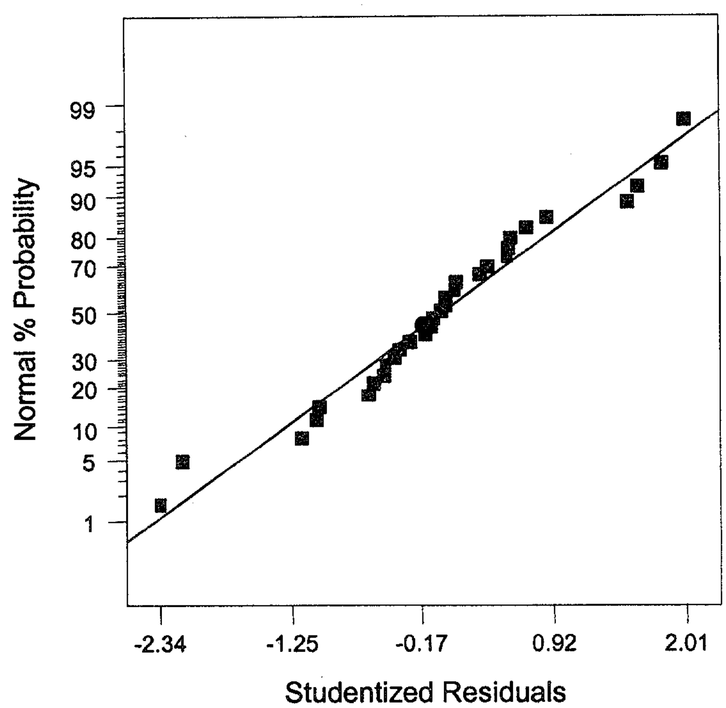


Figure B-21. Factorial experiment: normal probability plot for 28-day strength

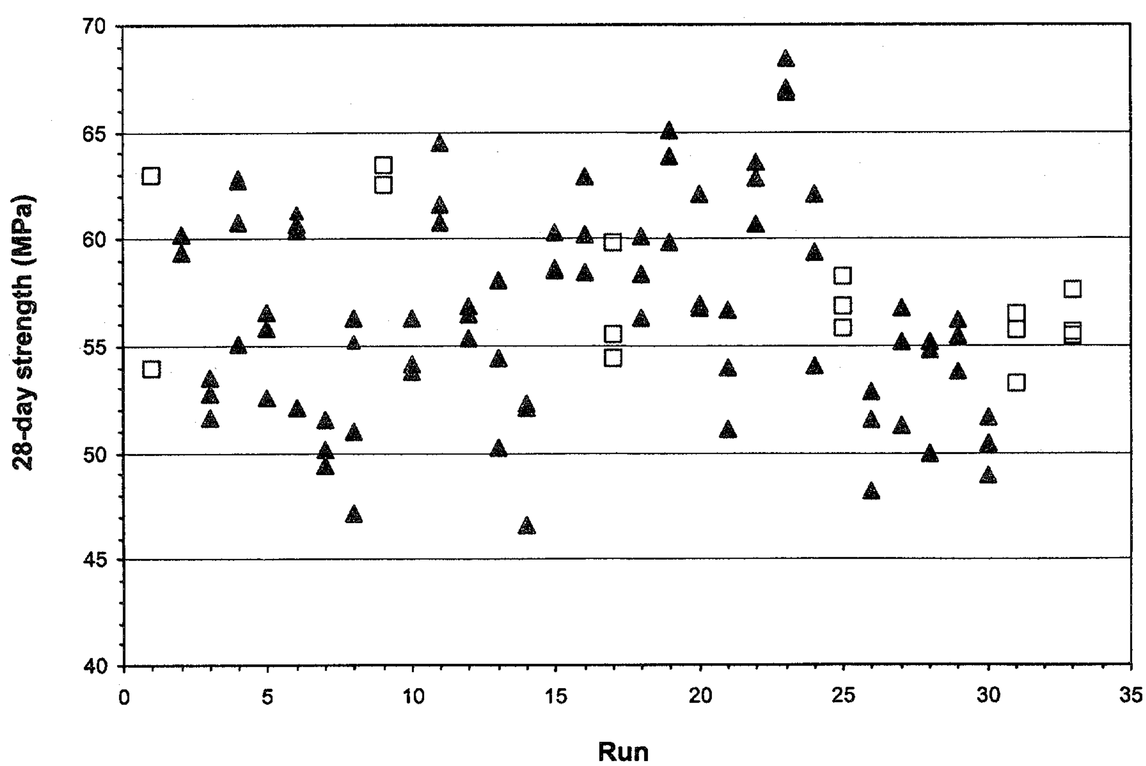


Figure B-22. Factorial experiment: raw data plot for 28-day strength (hollow squares indicate control runs)

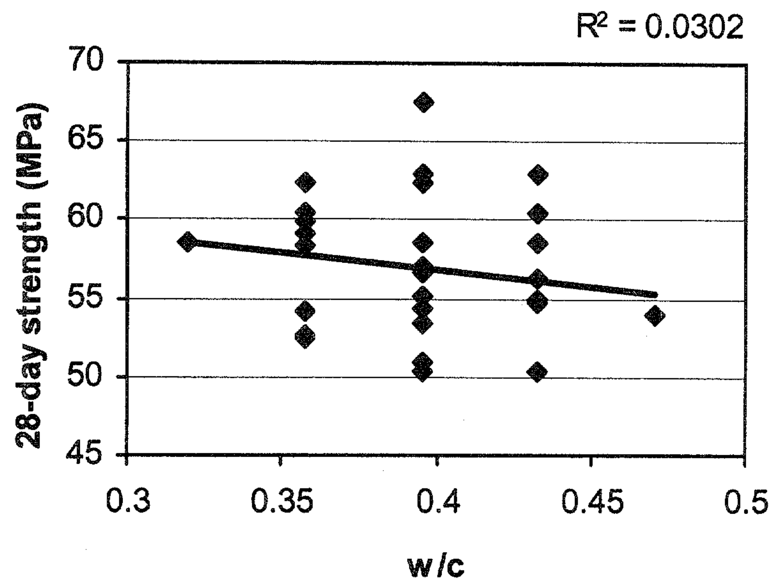


Figure B-23. Factorial experiment: scatterplot of 28-day strength vs. w/c

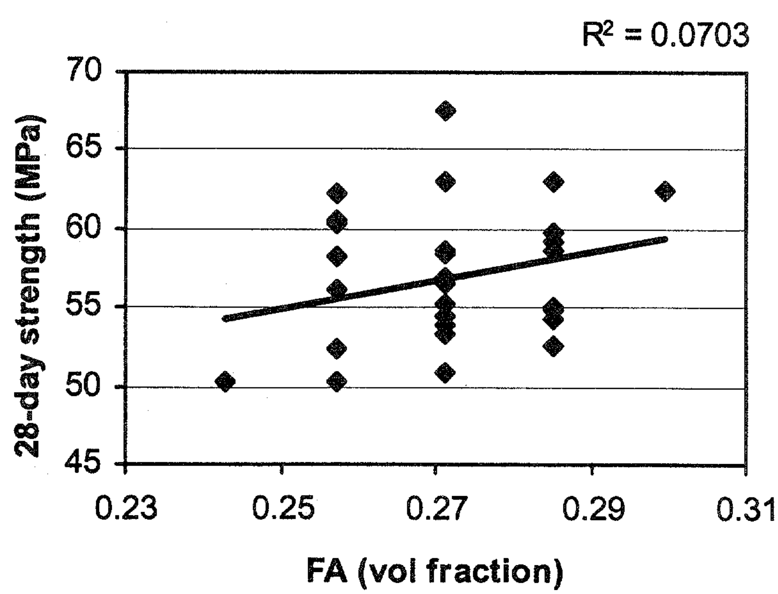


Figure B-24. Factorial experiment: scatterplot of 28-day strength vs. fine aggregate

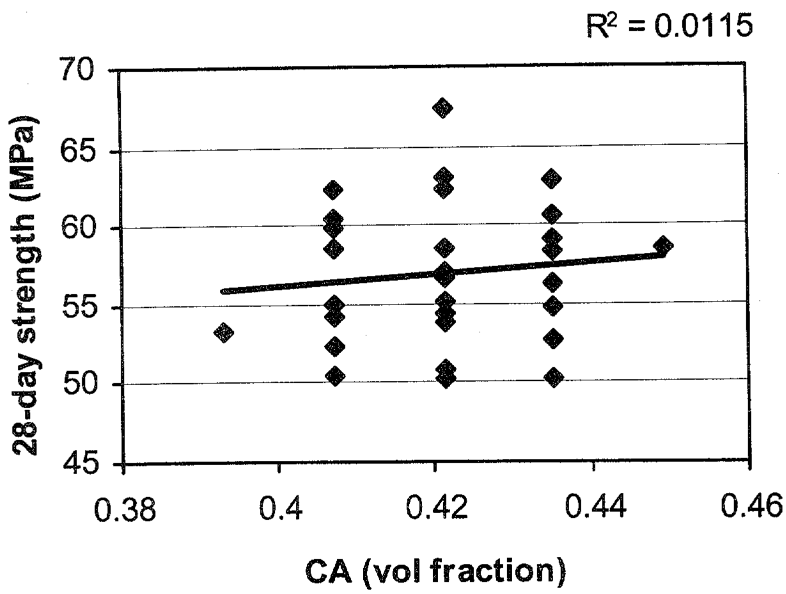


Figure B-25. Factorial experiment: scatterplot of 28-day strength vs. coarse aggregate

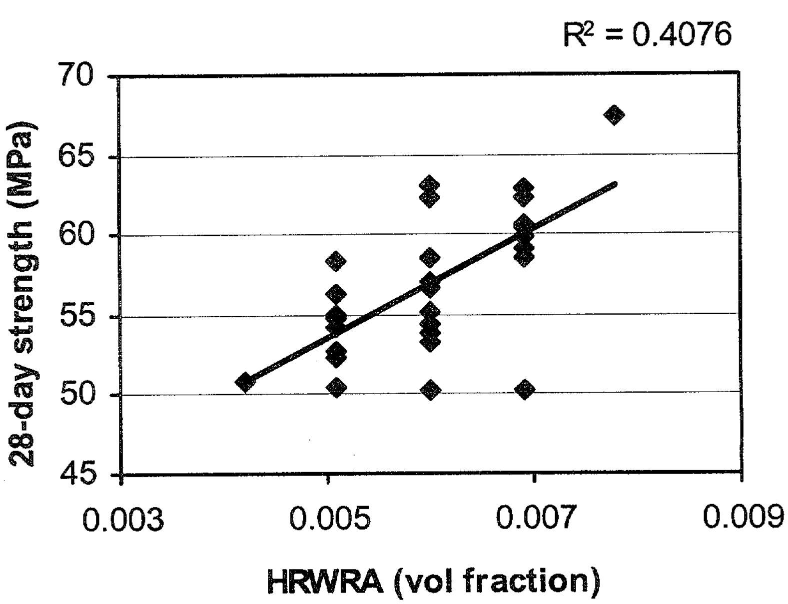


Figure B-26. Factorial experiment: scatterplot of 28-day strength vs. HRWRA

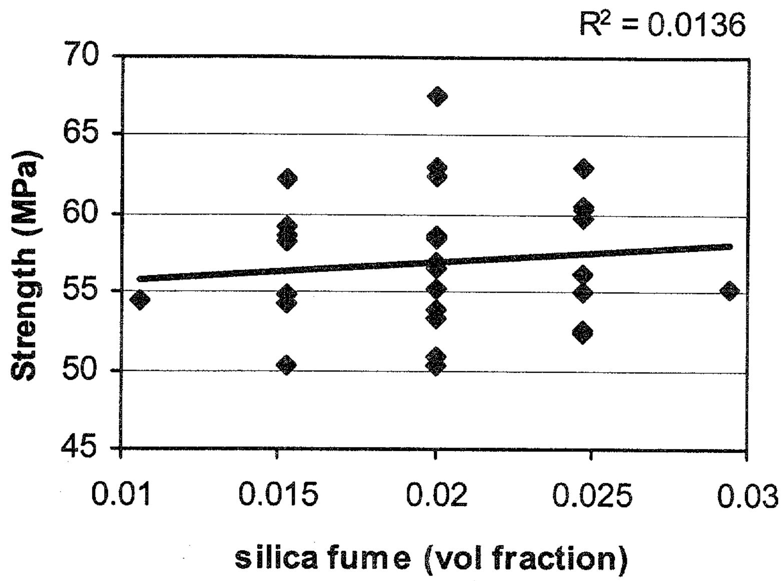


Figure B-27. Factorial experiment: scatterplot of 28-day strength vs. silica fume

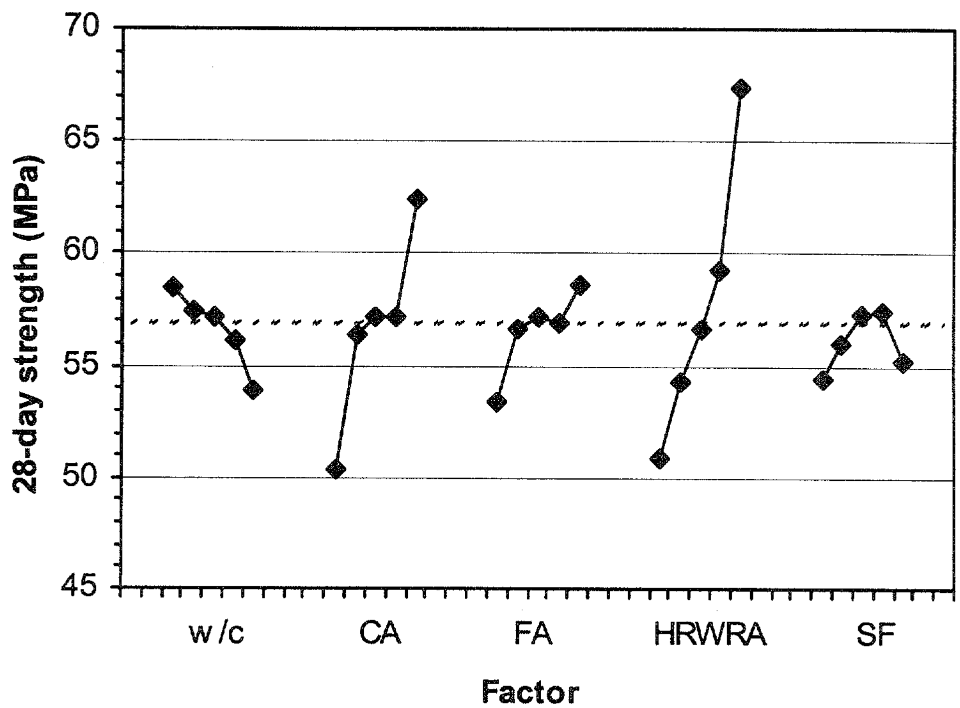


FIgure B-28. Factorial experiment: means plot for 28-day strength

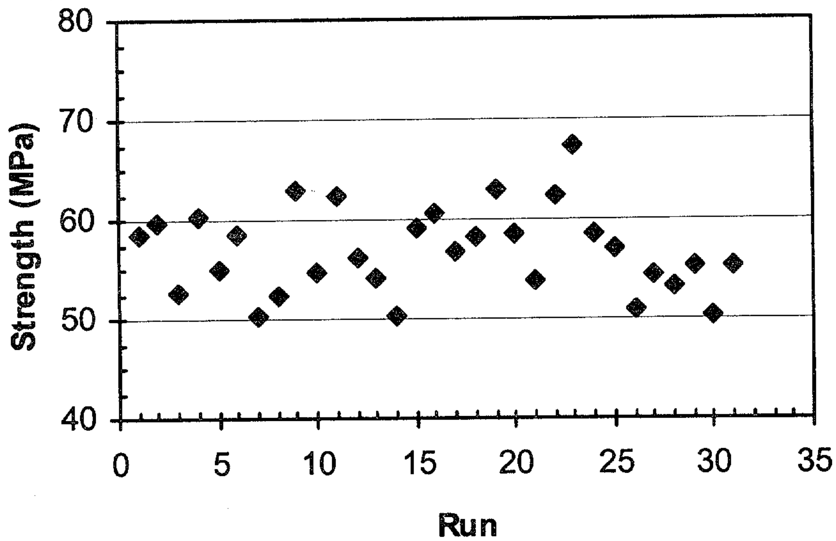


Figure B-29. Factorial experiment: 28-day strength vs. run sequence

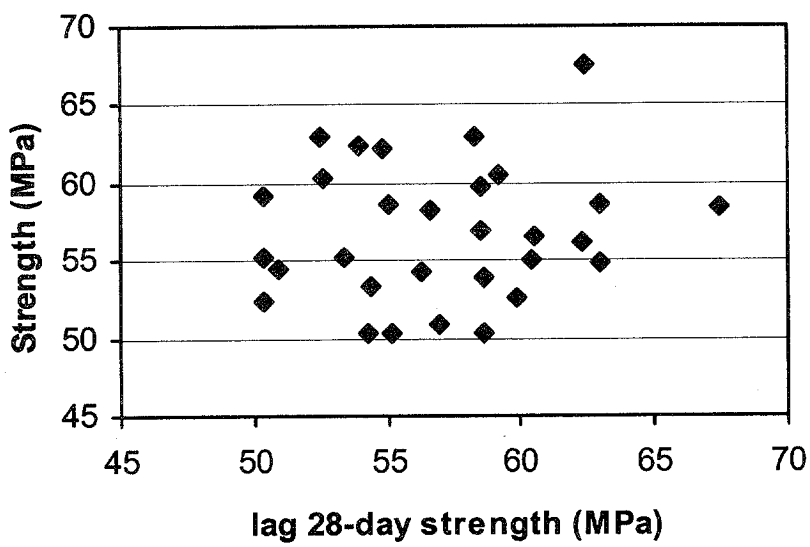


Figure B-30. Factorial experiment: lag plot for 28-day strength

B.2.4 RCT Charge Passed (coulombs)

Table B-19. Factorial experiment: sequential model sum of squares for RCT charge passed

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Mean	3155867	1	3155867	–	–
Linear	393517.2	5	78703.43	27.43	< 0.0001
2FI	15156.50	10	1515.65	0.40	0.9252
Quadratic	44410.76	5	8882.15	7.31	0.0040
Cubic (aliased)	10046.83	5	2009.37	4.77	0.0557
Residual	2104.61	5	420.92	–	–
Total	3621103	31	116809.8	–	–

Table B-20. Factorial experiment: lack-of-fit test for RCT charge passed

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Linear	69614.70	21	3314.99	6.30	0.0432
2FI	54458.20	11	4950.75	9.41	0.0221
Quadratic	10047.44	6	1674.57	3.18	0.1410
Cubic (aliased)	0.61	1	0.61	.001	0.9745
Pure error	2104.00	4	526.00	–	–

Table B-21. Factorial experiment: ANOVA for RCT charge passed model

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	441455.3	6	73575.89	74.25	< 0.0001
A	81666.67	1	81666.67	82.42	< 0.0001
B	6868.17	1	6868.17	6.93	0.0146
C	11440.67	1	11440.67	11.55	0.0024
E	292604.2	1	292604.2	295.30	< 0.0001
E^2	38369.41	1	38369.41	38.72	< 0.0001
AE	10506.25	1	10506.25	10.60	0.0034
Residual	23780.54	24	990.86	–	–
Lack of fit	21676.54	20	1083.83	2.06	0.2537
Pure error	2104.00	4	526.00	–	–
Cor total	465235.9	30	–	–	–

Table B-22. Factorial experiment: summary statistics for RCT charge passed model

Std. Dev.	31.48	R-Squared	0.9489
Mean	319.06	Adj R-Squared	0.9361
C.V.	9.87	Pred R-Squared	0.8784
PRESS	56577.00	Adeq Precision	34.166

Table B-23. Factorial experiment: coefficient estimates for RCT charge passed model

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High
Intercept	291.11	1	7.22	276.20	306.01
A (w/c)	58.33	1	6.43	45.07	71.59
B (fine agg)	-16.92	1	6.43	-30.18	-3.66
C (coarse agg)	-21.83	1	6.43	-35.09	-8.57
E (silica fume)	-110.42	1	6.43	-123.68	-97.16
E^2	36.11	1	5.80	24.14	48.09
AE	-25.63	1	7.87	-41.87	-9.38

Model equation for RCT charge passed in terms of coded factors:

$$\text{RCT charge passed} = 291.11 + 58.33{*}A - 16.92{*}B - 21.83{*}C - 110.42{*}E + 36.11{*}E^2 - 25.63{*}A{*}E$$

Model equation for RCT charge passed in terms of actual factors:

$$\text{RCT charge passed} = 635.4 + 4445.6{*}\text{w/c} - 1199.8{*}\text{fine agg} - 1548.5{*}\text{coarse agg} - 31651{*}\text{silica fume} + 1.635 \times 10^6{*}(\text{silica fume})^2 - 1.448 \times 10^5{*}\text{w/c}{*}\text{silica fume}$$

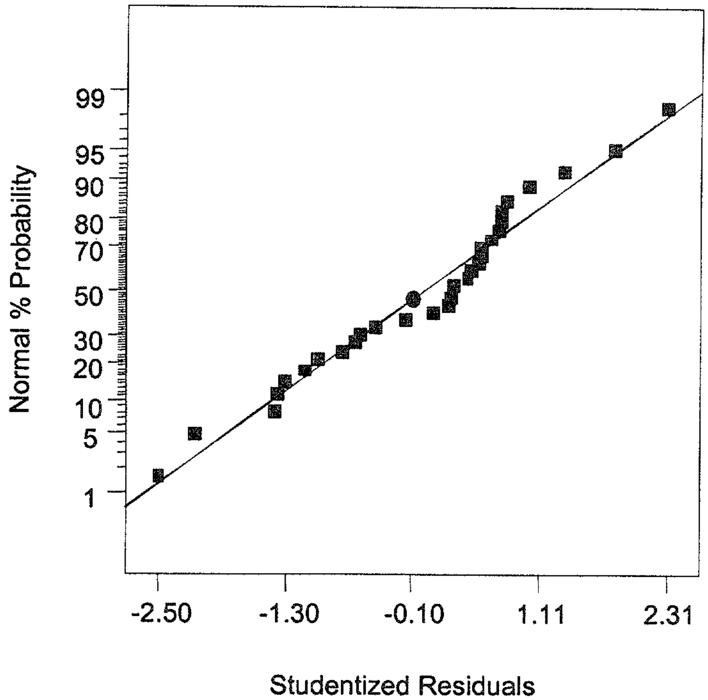


Figure B-31. Factorial experiment: normal probability plot for RCT charge passed

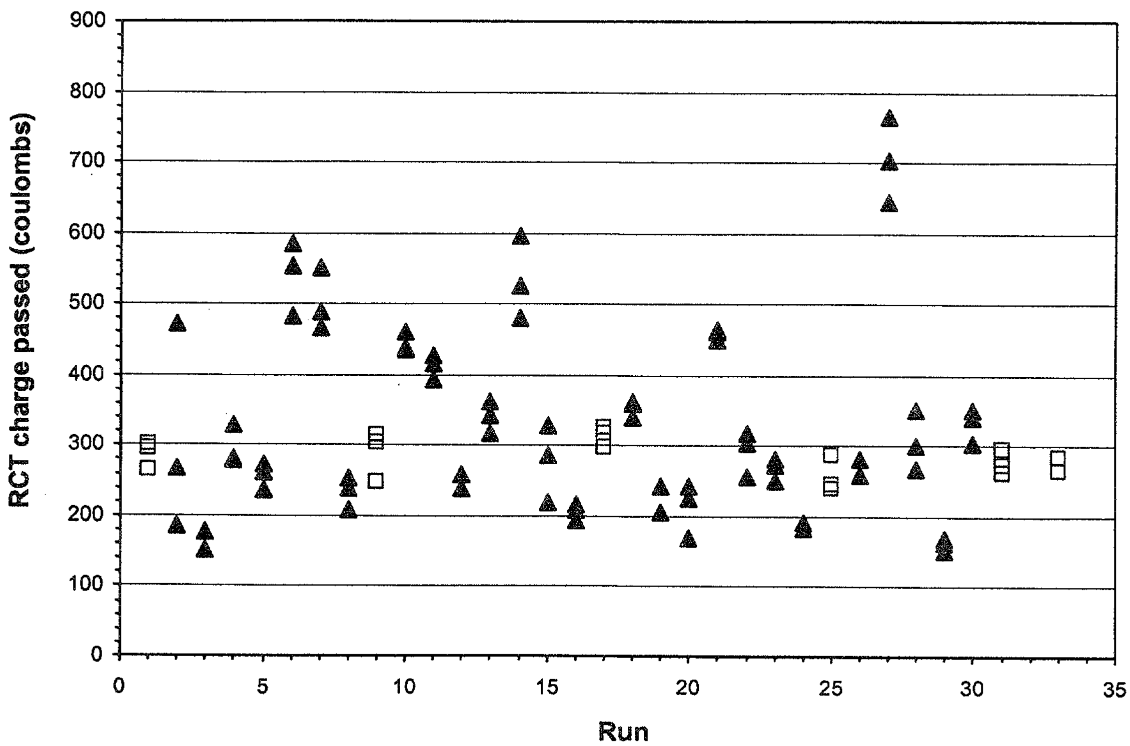


Figure B-32. Factorial experiment: raw data plot for RCT charge passed (hollow squares indicate control runs)

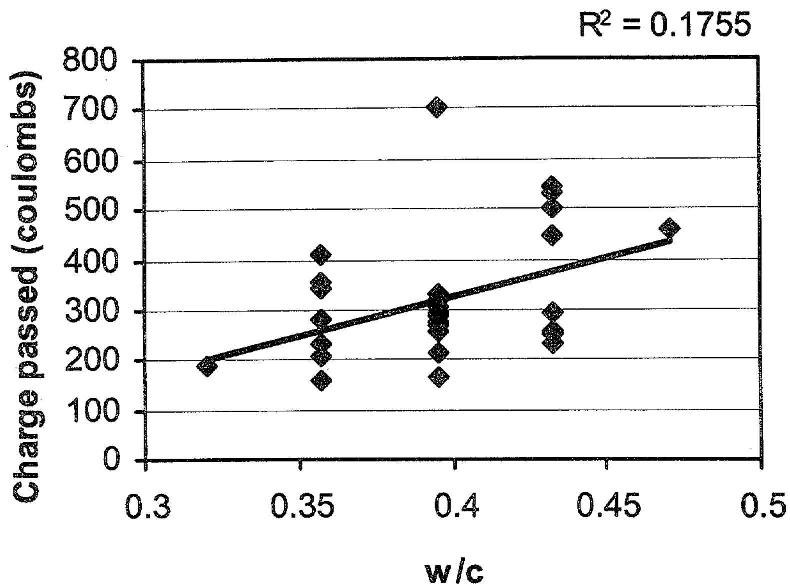


Figure B-33. Factorial experiment: scatterplot of RCT charge passed vs. w/c

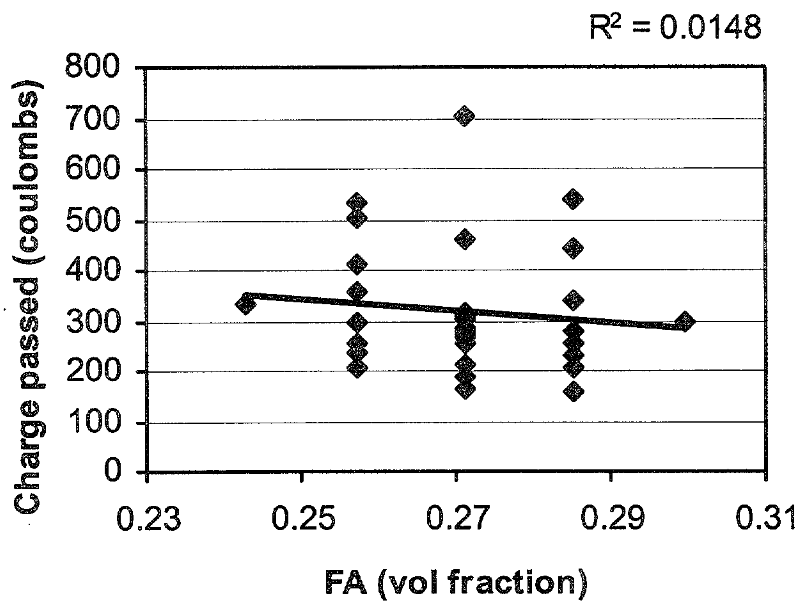


Figure B-34. Factorial experiment: scatterplot of RCT charge passed vs. fine aggregate

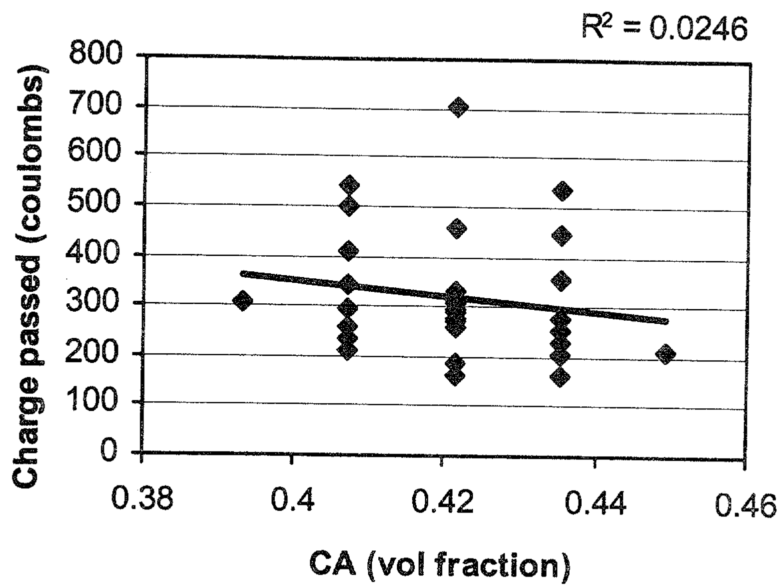


Figure B-35. Factorial experiment: scatterplot of RCT charge passed vs. coarse aggregate

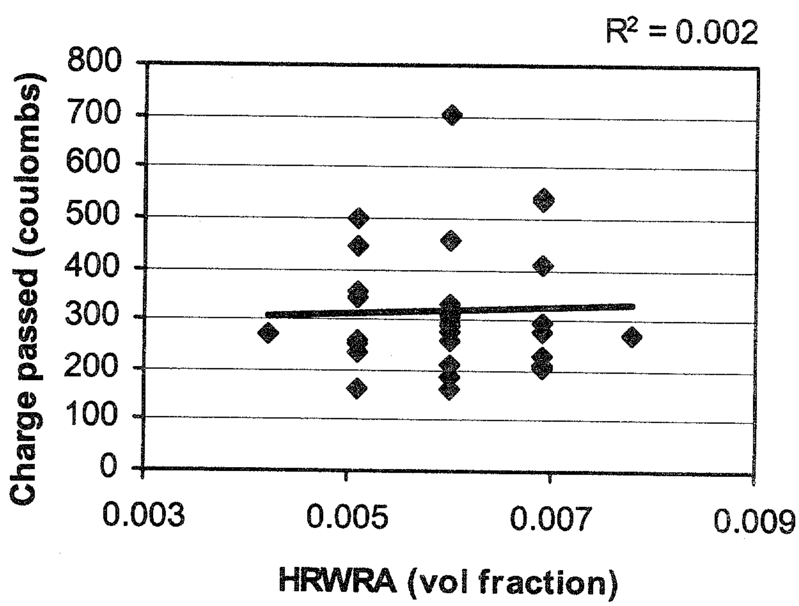


Figure B-36. Factorial experiment: scatterplot of RCT charge passed vs. HRWRA

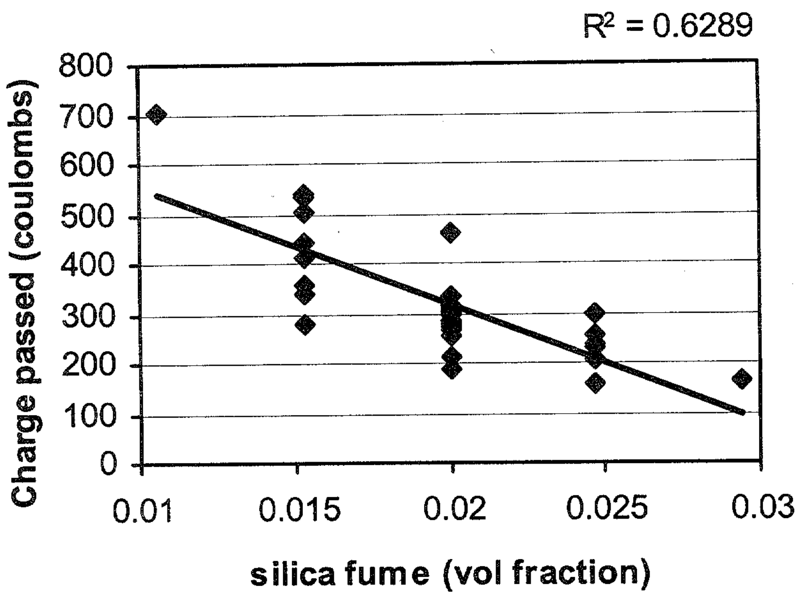


Figure B-37. Factorial experiment: scatterplot of RCT charge passed vs. silica fume

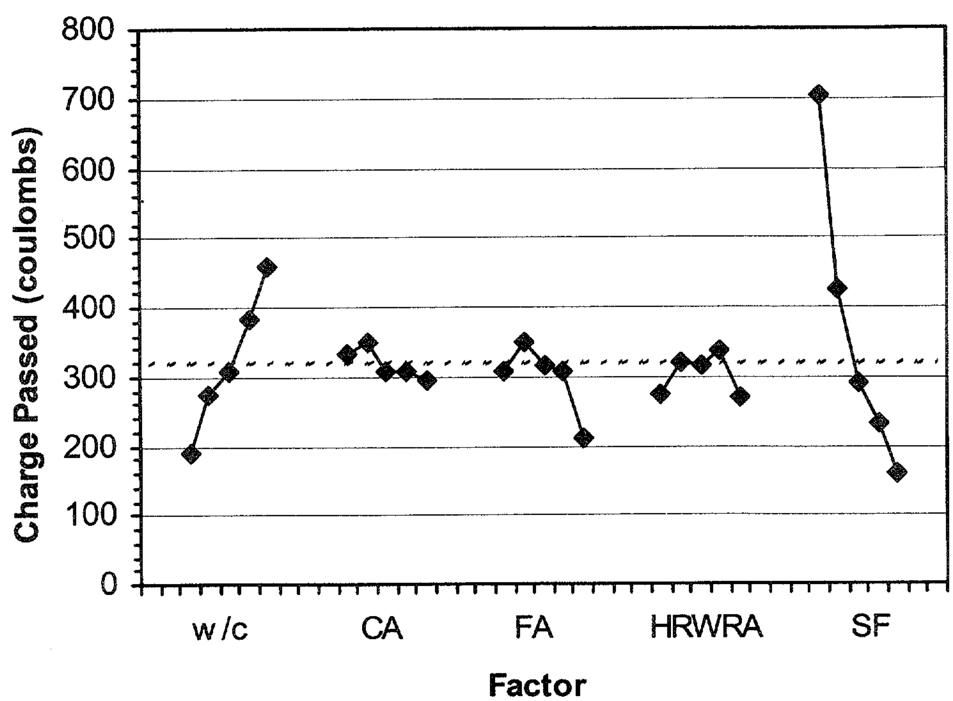


Figure B-38. Factorial experiment: means plot for RCT charge passed

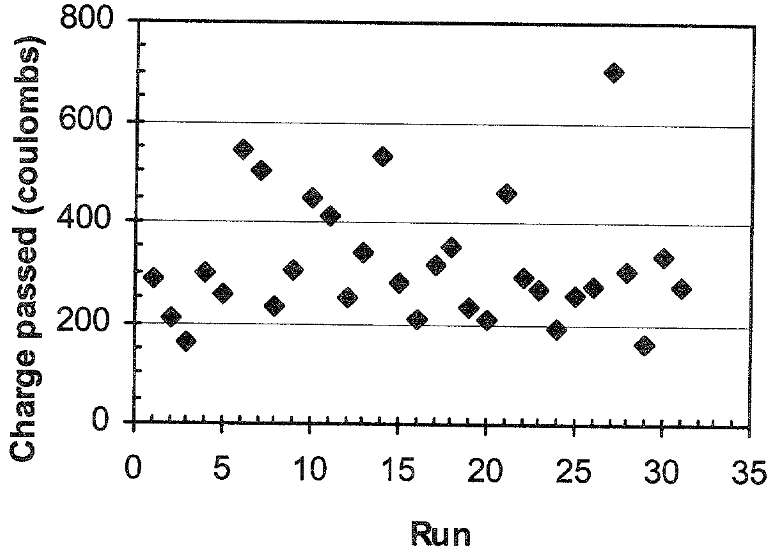


Figure B-39. Factorial experiment: RCT charge passed vs. run sequence

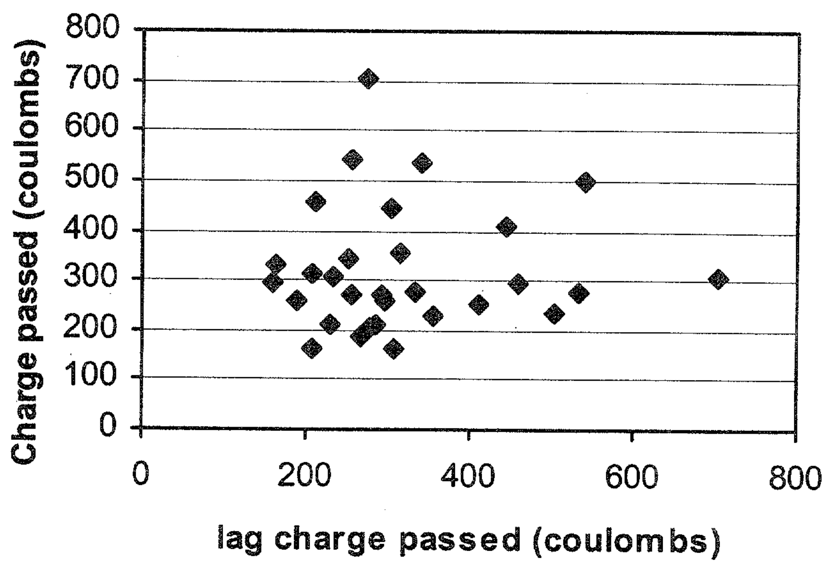


Figure B-40. Factorial experiment: lag plot for RCT charge passed

APPENDIX C. COST User's Guide

U. S. Department of Transportation
Federal Highway Administration

NIST
National Institute of Standards and Technology

Concrete Optimization Software Tool

USER'S GUIDE

July, 2001

Marcia J. Simon
Dale P. Bentz
James J. Filliben

ABSTRACT

This user's guide provides instructions for and examples of using the Concrete Optimization Software Tool (COST), a joint product of the Federal Highway Administration and the National Institute of Standards and Technology. COST provides an Internet-based system for optimizing concrete performance based on statistical experiment design and analysis methods. Working with local raw materials, COST designs an experimental program of concrete mixtures to be prepared and evaluated. In these mixtures, the user can vary the water-to-cement (w/c) ratio and other concrete mixture parameters such as the cement, mineral and chemical admixture, and aggregate contents. Once the measured responses (properties) for the prepared concretes are input into the COST system, it analyzes the results and determines the optimum mixture proportions based on user-supplied performance criteria. Results and analysis are provided in both graphical and numerical formats to aid in interpretation. Typical uses of COST might be to design a concrete that meets all specifications at minimum cost or to design a concrete that provides maximum durability within a specific cost range.

Keywords: Building technology, concrete, experiment design, mixture proportioning, optimization, response surfaces.

SECTION 1
Overview

C1.1 Introduction

In the simplest case, portland cement concrete is a four-component mixture of water, portland cement, fine aggregate, and coarse aggregate. Additional components, such as chemical admixtures (air entraining agents, superplasticizers) and mineral admixtures (coal fly ash, silica fume, blast furnace slag), may be added to the basic mixture to enhance certain properties of the fresh or hardened concrete. High-performance concrete mixtures, which may be required to meet several performance criteria (e.g., compressive strength, elastic moduli, rapid chloride permeability) simultaneously, typically contain at least six components. Thus, optimizing mixture proportions for high-performance concrete, which contains many constituents and is often subject to several performance constraints, can be a difficult and time-consuming task.

The Concrete Optimization Software Tool (COST) is an online interactive system developed to assist engineers, concrete producers, and researchers in optimizing portland cement concrete mixtures for their particular applications. COST applies response surface methodology (RSM), a collection of statistical experiment design and analysis methods, to the problem of optimizing concrete mixture proportions. RSM is often used in industry for product development, formulation, and improvement, and is applicable to problems such as concrete mixture proportioning where several input variables (factors) influence a performance measure (response).

COST is intended to provide an introduction to concrete practitioners who are unfamiliar with the concepts and process of applying RSM to concrete mixture proportioning. COST allows users to learn how RSM can be applied to the problem of optimizing concrete mixtures.

There are two scenarios for which COST could be applied:

1. The first, and probably most common, would be the case where a user wants to proportion a concrete mixture to meet a set of specifications at minimum material cost.

2. The second is the case where the user wants to maximize (or minimize) a particular response or responses, irrespective of cost.

COST can be used to optimize cement paste, mortar, or concrete mixtures. In all three cases, varying the mixture component proportions affects both fresh and hardened properties of the paste, mortar or concrete. The properties (responses) depend on the proportions of the components. Table C-1 lists examples of typical components and responses for concrete mixtures (components and responses other than those listed can be used).

In COST, the water-cement (w/c) ratio (or water-cementitious materials (w/cm) ratio) is varied along with up to four additional components. These are referred to as variable factors. Other factors may be included in the mixture at fixed (constant) levels, and are referred to as fixed factors. Up to five concrete properties, or responses, (e.g., slump, strength, air content, cost, etc.)

can be designated by the user according to the requirements of the application. These concepts are explained more fully in section 2.

Table C-1. Examples of components and responses

Components	Responses
Water **Cement** (including blended cements) **Mineral admixtures** (e.g., fly ash, silica fume, slag, metakaolin) **Chemical admixtures** (water reducers, retarders, air entraining agents) **Aggregate**	**Fresh properties** (e.g., slump, air content, unit weight, temperature, set time) **Mechanical properties** (e.g., strength, modulus of elasticity, shrinkage, creep) **Durability** (e.g., freeze-thaw, scaling, alkali silica reaction, sulfate attack, abrasion)

COST is accessible via the Internet. The program consists of a front-end HTML interface that allows the user to enter required information. Underlying code (written in C) processes the input, generates the experiment designs and mixture proportions, calls routines for statistical analysis, and generates output. The statistical analysis routines are part of an interactive statistical software package, DATAPLOT, which was developed at the National Institute of Standards and Technology (NIST).

C1.2 Scope

COST is not intended to supplant or compete with commercially available experiment design and analysis software packages. Rather, the purpose of COST is to introduce to the concrete practitioner the concepts of statistical experiment design and analysis using RSM and how they might be applied to concrete mixture proportioning. *COST is specifically geared toward the application of these methods to concrete mixture proportioning.*

This section provides a general overview of the COST program. Section 2 of this manual provides step-by-step instructions for using COST. Section 3 contains a glossary of terms, additional details on the statistical aspects of the experiment designs and analyses used, and a list of references.

C1.3 System Requirements

To use COST, your system must have the following components and settings:

- Personal computer (Pentium®[1] or equivalent) with video card and monitor set for 800 x 600 resolution (min) and 65536 colors.

[1] Certain commercial products are identified to completely specify the COST system. In no case does such identification imply endorsement by NIST or the FHWA or that the identified products are the best available for the purpose.

- Access to the Internet (World Wide Web) and one of the following browsers: Netscape Navigator 4.0 (or above) or Microsoft® Internet Explorer 4.0 (or above). The COST interface uses both frames and JavaScript.

C1.4 Disclaimer

This software was developed at NIST by employees of the Federal Government in the course of their official duties. Pursuant to Title 17, Section 105 of the U.S. Code, this software is not subject to copyright protection and is in the public domain. COST is an experimental system. NIST and the Federal Highway Administration (FHWA) assume no responsibility whatsoever for its use by other parties, and make no guarantees, expressed or implied, about its quality, reliability, or any other characteristic. We would appreciate acknowledgement if the software is used.

The U.S. Department of Commerce and the U.S. Department of Transpotation make no warranty, expressed or implied, to users of COST and associated computer programs, and accepts no responsibility for its use. Users of COST assume sole responsibility under Federal law for determining the appropriateness of its use in any particular application; for any conclusions drawn from the results of its use; and for any actions taken or not taken as a result of analyses performed using these tools.

Users are warned that COST is intended for use only by those competent in the field of concrete technology and is intended to supplement the informed judgment of the qualified user. Lack of accurate predictions by the COST models could lead to erroneous conclusions with regard to materials selection and design. All results should be evaluated by an informed user.

C1.5 General Information

C1.5.1 COST Homepage and Main Menu

The COST homepage may be accessed at http://ciks.cbt.nist.gov/cost. The COST homepage is shown in figure C-1.

The homepage contains a brief overview of the COST program. The blue bar on the left side of the screen is the main menu. Menu selections are described briefly below. Details on each step are provided in section 2, "Using COST."

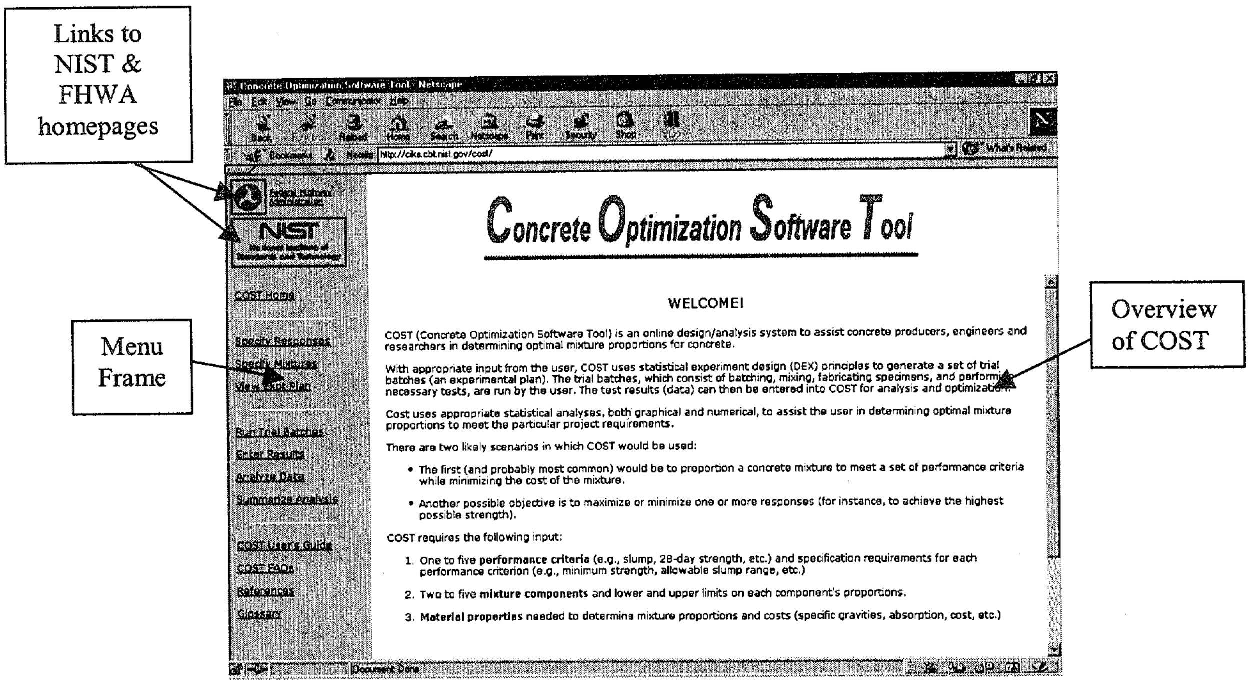


Figure C-1. COST homepage

COST Home—allows user to return to the initial screen (figure C-1) at any time.

Specify Responses—user enters information on responses to be measured. Responses are the measured properties of the concrete (fresh or hardened) such as slump, air content, strength, shrinkage, etc., that are specified for the particular project.

Specify Mixtures—user enters information on mixture components and proportions, and COST generates an experimental plan.

View Experimental Plan—user can view a previously generated experimental plan.

Run Trial Batches—contains guidelines for performing the trial batches according to the experimental plan. This step is performed by the user in his/her laboratory, and involves batching, fabricating, curing, and testing specimens. Types of specimens and test methods used will depend on the responses specified in step 1. It is the user's responsibility to determine the appropriate test method to use.

Enter Results—user enters test results for each trial batch and each response.

Analyze Data—COST provides 10 analysis tasks to assist the user in analyzing and interpreting the results. The tasks include checking the experiment design, looking at trends in the data graphically, generating empirical (quadratic) models for each response, and optimizing according to individual runs, means, and models.

Summarize Analysis—summary of main results of analysis.

User's Guide—HTML version of the COST User's Guide. A PDF version is also available for download.

FAQ's—frequently asked questions.

References—a list of references on statistics, response surface methods and DATAPLOT (software used by COST).

Glossary—a glossary of statistical terms.

SECTION 2
Using COST

C2.1 Background and Preliminary Planning

Using COST requires several steps, including planning, running trial batches, entering results, analyzing, interpreting, and summarizing results. These tasks have been divided into the following six steps (as listed in the COST menu):

- Specify responses.
- Specify mixtures.
- Run trial batches.
- Enter results.
- Analyze data.
- Summarize analysis.

In most cases, these steps will be performed in the order listed above. Each step is described in detail in the sections below.

Before starting the six-step process, the user must perform some preliminary steps:

1. Define the overall objective of the project. Typical objectives include the following:

    - Minimize cost while meeting several performance criteria for responses.
    - Minimize or maximize a single response or several responses.

2. Define the properties (responses) and mixture components (factors) to be included, and define which will be variable or fixed factors. Variable factors include w/c or w/cm plus up to four additional components. Additional factors may be included at fixed levels. See "Background Information" below for further details.

3. Define the performance criteria (most likely based on the job specifications) for each response, and the numerical ranges for each factor.

4. Collect necessary material information (e.g., properties and costs of each component). The required information for each type of material is listed in table C-2.

C2.1.1 Responses

Responses are the concrete properties of interest that will be measured and compared to specified performance criteria (i.e., limits on allowable values of the responses). The responses are dependent variables; that is, the value of a measured response depends on the settings of the independent variables, or factors (see step 2 below). Responses and performance criteria are often dictated by specifications. For example, the specifications for a particular job may indicate that the concrete must have a slump between 50 mm and 100 mm, an air content between 4.5 percent and 7.5 percent by volume, and 28-day strength greater than 69 MPa. The responses in this case are slump, air content and 28-day strength, and the performance criteria are the ranges of acceptable values of the responses.

C2.1.2 Factors

The factors are the independent variables that affect the measured values of the responses. For concrete mixtures, these factors include mixture proportions (relative amounts of each component material) as well as others related to construction practice and environmental conditions. COST assumes that construction and environmental conditions are fixed (as in the case of a set of laboratory or plant trial batches), so *the factors of concern are the mixture proportions for each component.*

Concrete can contain a variety of component materials. Allowable material types for this version of COST include the following:

- Water.
- Cement.
- Mineral admixtures (up to 4): fly ash, silica fume, slag, other (user specified).
- Chemical admixtures (up to 3): all user specified.
- Aggregates (up to 3): coarse, fine, other (user specified).

COST always requires that either w/c or w/cm be included as a variable factor. Thus, the two mixture components water and cement are accounted for in this single factor.

Factors may be variable or fixed (set at a constant level). For concrete mixture proportioning, variable factors would usually be the mixture components expected to have the most significant effects on the responses. Fixed factors would be those expected to have little or no effect, and would be held constant in the experiment. Any of the factors included in COST may be set as variable or fixed; however, COST limits the user to a maximum of five variable factors for any one experiment (the greater the number of variable factors, the greater the number of trial batches required). Because w/c or w/cm is always considered to be one factor, up to six material components (water, cement, and four others) may be varied.

For all variable factors, low and high settings, or levels, must be defined. The low and high settings are the range over which the factor will vary. For example, w/c could have a range of 0.35 (low level) to 0.45 (high level), or silica fume could have a range of 5 to 10 percent (cement mass replacement). For fixed factors, a fixed (constant) level is specified.

Table C-2 summarizes the information required for different types of materials.

Once the user has decided on the factors to include, defined their ranges (for variable factors) or constant levels (for fixed factors), and obtained other necessary information (table C-2), the information may be entered into COST to generate a trial batch plan.

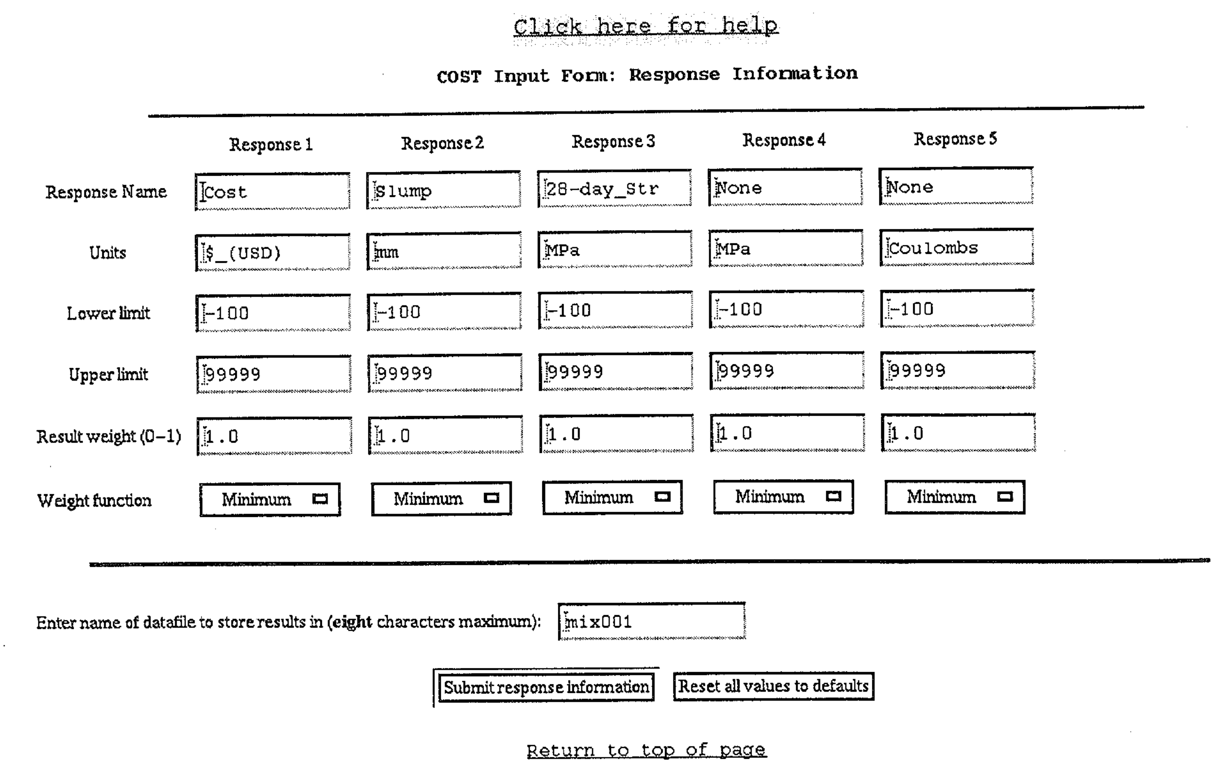
In most cases, the selection of components and their ranges is up to the user; however, in some cases, some of the factors and levels may be designated in specifications. For example, a specification may have a maximum w/c, or minimum silica fume content. COST does not provide guidance on the selection of minimum and maximum values for the components.

Table C-2. Information required for different materials

Material	Information Required
Water	None
Cement	Specific gravity Cost ($/kg)
Mineral admixture	Replacement rate (percent mass fraction of cement) Specific gravity Cost ($/kg)
Chemical admixture	Dosage rate (liters per kg cement) Specific gravity Percent solids (by mass fraction) Cost ($/liter)
Aggregates	Volume fraction (or mass fraction) Specific gravity Absorption (%) Moisture content (%) Cost ($/kg)

C2.2 Step 1—Specify Responses

When "Specify Responses" is selected from the main menu, a form entitled "COST Input Form: Response Information" appears in the right frame. This form is shown in figure C-2.


Click here for help

COST Input Form: Response Information

	Response 1	Response 2	Response 3	Response 4	Response 5
Response Name	Cost	slump	28-day_str	None	None
Units	$_(USD)	mm	MPa	MPa	Coulombs
Lower limit	-100	-100	-100	-100	-100
Upper limit	99999	99999	99999	99999	99999
Result weight (0–1)	1.0	1.0	1.0	1.0	1.0
Weight function	Minimum	Minimum	Minimum	Minimum	Minimum

Enter name of datafile to store results in (eight characters maximum): mix001

Submit response information | Reset all values to defaults

Return to top of page

Figure C-2. "Response Information" form

Referring to figure C-2, the following information must be entered into COST for each response:

- A **name** for the response. The name should be as short as possible (no more than 10 characters) and may include alphanumeric characters and underscores (e.g., slump, 28-day_str). No other characters are allowed.

- The **units** in which the response is measured.

- A **lower limit** for the response, if applicable. This would be a specified minimum value (e.g., minimum 1-day strength of 15 MPa). If there is not a lower limit for the response, a default value of –100 is used.

- An **upper limit** for the response, if applicable. This would be a specified maximum value (e.g., maximum rapid chloride permeability (RCT) test result of 1000 coulombs). If there is no upper limit, a default value of 99999 is used.

- A **result weight factor** between 0 and 1, to indicate the relative importance of the response in optimization, compared to the other responses. A factor of 1 indicates most important. The default value is 1 for all responses. If all responses are of equal importance, use the default values. (*Note: to optimize a single response while ignoring all others, set the weight factor of the response of interest to 1 and the weight factors of all others to zero*).

- The **type of weight function** to use in optimization. Choices are:

  - Minimum value is best (linear decreasing from 1 to 0 over response range).
  - Maximum value is best (linear increasing 0 to 1 over response range).
  - Target value is best (linear increasing from 0 to 1 over lower half of response range, and decreasing from 1 to 0 over upper half of response range).
  - Within range (all values in range are equally acceptable but no values outside range are acceptable).

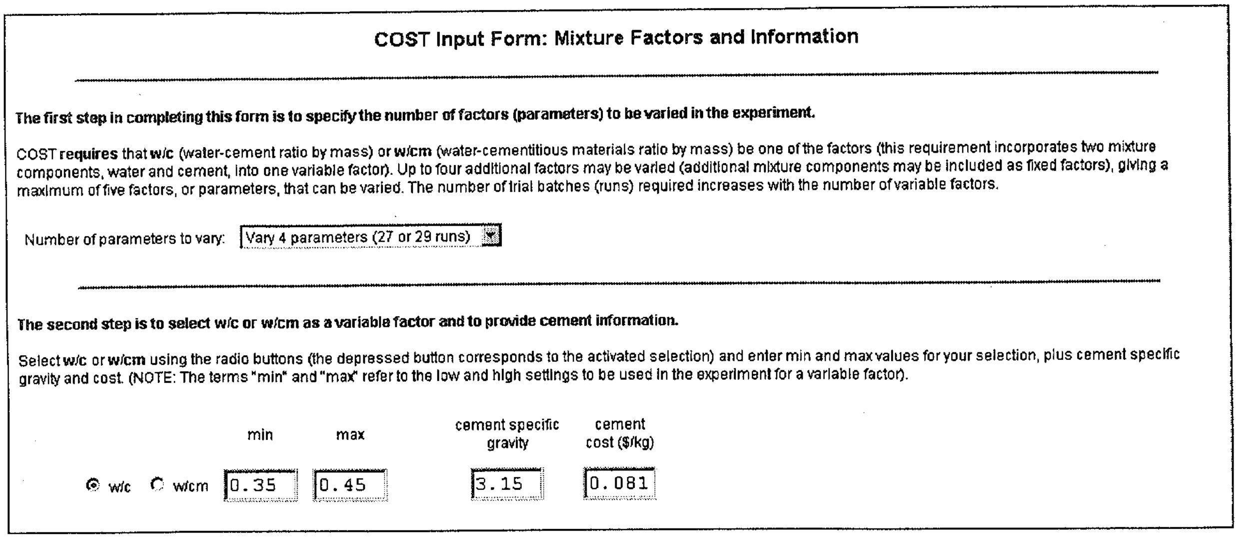
  The response range is defined by the lower and upper limits specified above, or by the minimum (or maximum) value of the response obtained in the experiment if it is greater than (less than) the lower (upper) limit. A different type of weight function can be specified for each response, if desired.

- A **filename** for the project, **eight** characters or fewer (alphanumeric characters only) and <u>no extension</u>. The filename will be unique to a particular project, and COST will create several files using the same filename with different extensions as you proceed through the steps (*Note: remember this filename, as it will be needed in subsequent steps as well*).

After entering the filename, the user should click on "Submit" to submit the completed form information to COST, or "Reset" to reset all settings to their default values.

C2.3 Step 2—Specify Mixtures

When "Specify Mixtures" is selected from the main menu, a form entitled "COST Input Form: Mixture Factors and Information" appears. Figure C-3 shows the first two sections of this form. The instructions for completing these sections are listed below.



COST Input Form: Mixture Factors and Information

The first step in completing this form is to specify the number of factors (parameters) to be varied in the experiment.

COST **requires** that **w/c** (water-cement ratio by mass) or **w/cm** (water-cementitious materials ratio by mass) be one of the factors (this requirement incorporates two mixture components, water and cement, into one variable factor). Up to four additional factors may be varied (additional mixture components may be included as fixed factors), giving a maximum of five factors, or parameters, that can be varied. The number of trial batches (runs) required increases with the number of variable factors.

Number of parameters to vary: Vary 4 parameters (27 or 29 runs)

The second step is to select w/c or w/cm as a variable factor and to provide cement information.

Select **w/c** or **w/cm** using the radio buttons (the depressed button corresponds to the activated selection) and enter min and max values for your selection, plus cement specific gravity and cost. (NOTE: The terms "min" and "max" refer to the low and high settings to be used in the experiment for a variable factor).

	min	max	cement specific gravity	cement cost ($/kg)
◉ w/c ○ w/cm	0.35	0.45	3.15	0.081

Figure C-3. First two sections of "Mixture Factors and Information" input form

C2.3.1 Instructions for Section 1: Number of Parameters (Factors) to Vary

In section 1, the number of parameters (factors) to vary is selected. The user may select 2 to 5 parameters to vary (default is 4). The number of experimental runs is also shown for each selection. The number of experimental runs depends on whether the user includes 3 or 5 center points in the design (the number of center points is entered at the bottom of the form).

- **To select the number of parameters** to vary, use the pulldown menu.

C2.3.2 Instructions for Section 2: Select w/c or w/cm

In section 2, the user selects w/c or w/cm as a factor, defines the range (low and high settings) for this factor, and enters information about the cement.

- **To select w/c or w/cm** , click on the radio button next to the desired choice.
- **Enter the low and high settings of w/c or w/cm** (by mass fraction) in the boxes labeled "min" and "max", respectively.
- **Enter the cement specific gravity.**
- **Enter the cement cost** in dollars per kilogram.

C2.3.3 Instructions for Section 3: Select Other Mixture Components

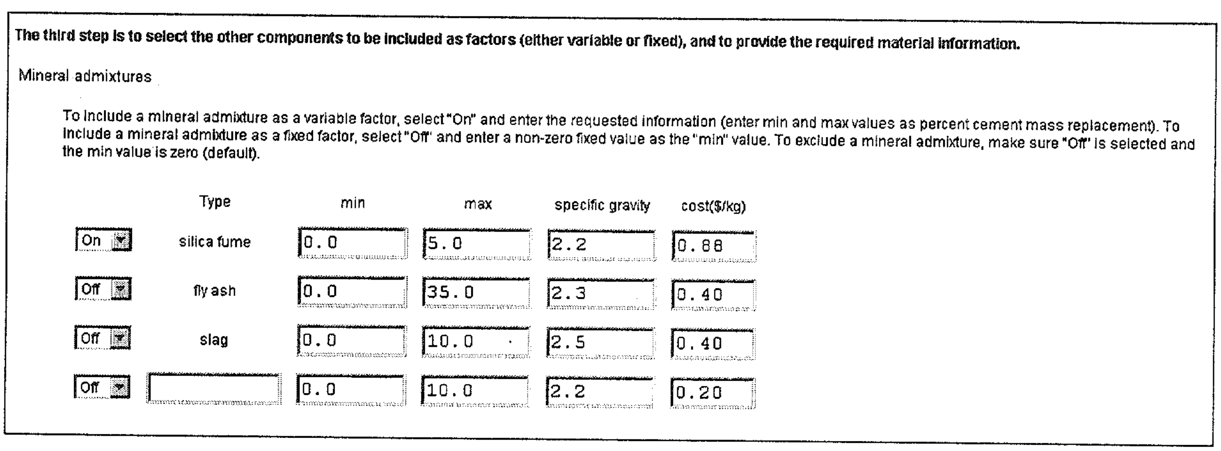
The third section of the form allows selection of other mixture components (mineral admixtures, chemical admixtures, and aggregates). A maximum of four additional variable factors, and any number of fixed factors, may be included. The total number of variable factors selected (including w/c or w/cm, selected in section 2) must match the "number of parameters to vary" selected in section 1.

The additional factors are selected from three types of materials: mineral admixtures, chemical admixtures, and aggregates. Regardless of type, the first task is to indicate whether the factor will be included or not, and if it will be included, whether it will be variable or fixed. This setting is defined using a pulldown menu on the left of the factor name, as described in the following instructions (refer to figure C-4 below):

- **To include a component as a variable factor**, select "On" in the pulldown menu at the left. Enter the type of material (if not predefined), the low and high settings in the "min" and "max" boxes, and the additional information in the other boxes.

- **To include a component as a fixed factor** (held at a constant level), select "Off" in the pulldown menu on the left, and enter a nonzero fixed setting in the "min" box (the entry in the "max" box will be ignored). Then enter the additional information for each fixed factor in the boxes.

- **To exclude a component completely**, select "Off" in the pulldown menu on the left, and set the value in the "min" box to zero. All other information for these factors is ignored. *NOTE: this is the default setting for all factors.*


The third step is to select the other components to be included as factors (either variable or fixed), and to provide the required material information.

Mineral admixtures

To include a mineral admixture as a variable factor, select "On" and enter the requested information (enter min and max values as percent cement mass replacement). To include a mineral admixture as a fixed factor, select "Off" and enter a non-zero fixed value as the "min" value. To exclude a mineral admixture, make sure "Off" is selected and the min value is zero (default).

	Type	min	max	specific gravity	cost($/kg)
On	silica fume	0.0	5.0	2.2	0.88
Off	fly ash	0.0	35.0	2.3	0.40
Off	slag	0.0	10.0	2.5	0.40
Off		0.0	10.0	2.2	0.20

Figure C-4. Third section of "Mixture Factors..." form (mineral admixtures section)

C2.3.4 Specific Instructions for Mineral Admixtures

There are three pre-designated mineral admixtures (fly ash, silica fume, and slag), plus one blank for a user-designated choice. Mineral admixtures ranges are defined in terms of percent cement mass replacement. Specific gravity and cost must also be entered.

- **Enter the name** of the mineral admixture (if the user-defined box is used).
- **To define the range for a mineral admixture**, enter the min and max values in units of percent cement mass replacement.
- **Enter the specific gravity** of the mineral admixture.
- **Enter the cost** of the mineral admixture in dollars per kilogram.

C2.3.5 Specific Instructions for Chemical Admixtures

All chemical admixtures are user-designated, and chemical admixtures ranges are defined in terms of dosage rate in liters per kg of cement.

Chemical admixtures

To include a chemical admixture as a variable factor, select "On" and enter the requested information (enter min and max values as dosage in liters per kg of cement). To include a chemical admixture as a fixed factor, select "Off" and enter a non-zero fixed value as the "min" value. To exclude a chemical admixture, make sure "Off" is selected and the min value is zero (default). **Please use underscores instead of spaces in the chemical admixture names.**

	Type	min	max	specific gravity	% solids (by mass)	cost ($/liter)
Off		0.0	1.0	1.0	50.0	0.20
Off		0.0	1.0	1.0	50.0	0.20
Off		0.0	1.0	1.0	50.0	0.20

Figure C-5. Third section of "Mixture Factors..." input form (chemical admixtures section)

- **Enter the name** of the chemical admixture.
- **To define the range for a chemical admixture**, enter the min and max values in units of dosage in liters per kilogram of cement (note that this is L/kg, not L/100 kg!!).
- **Enter the specific gravity** of the chemical admixture.
- **Enter the percent solids** (by mass fraction) of the chemical admixture.

- **Enter the cost** of the chemical admixture in dollars per liter.

C2.3.6 Specific Instructions for Aggregates

Aggregates include two predesignated types (coarse and fine), and one blank for a user-designated choice. The user-designated choice may be used for an additional aggregate or fibers. Aggregates may be defined in terms of volume fraction or mass fraction. Steps for entering aggregate information (see figure C-6) are as follows:

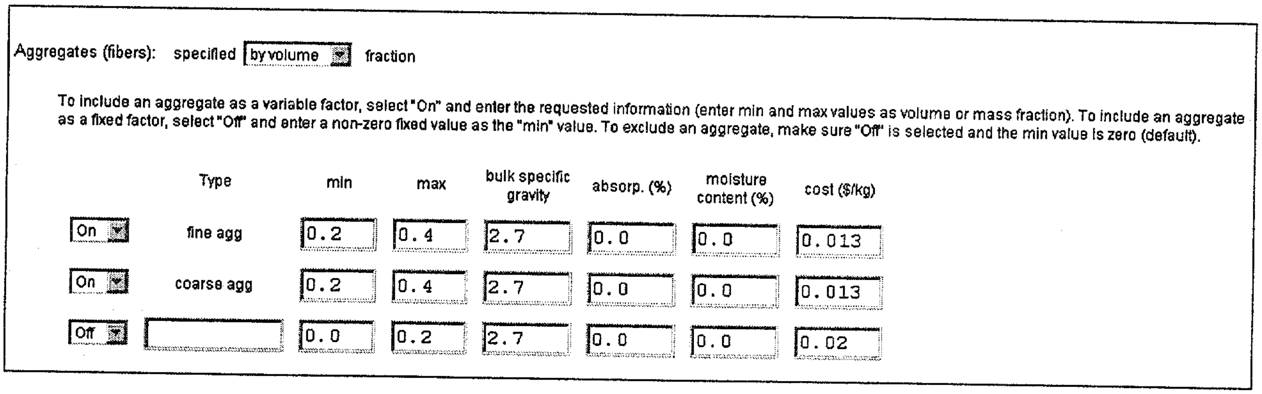


Figure C-6. Third section of "Mixture Factors..." form (aggregates section)

- **Select how the aggregate range will be defined** (by volume or by mass) using the pulldown menu at the top of the section (see figure 6).

- **Enter a name** for the aggregate (if the user-defined box is used).

- **To define the range for the aggregate**, enter the min and max values in units of volume fraction or mass fraction (depending on the selection made above).

- **Enter the bulk specific gravity** for the aggregate.

- **Enter the absorption** of the aggregate (in percent by mass of aggregate).

- **Enter the moisture content** of the aggregate as batched (in percent by mass of aggregate).

- **Enter the cost** of the aggregate in dollars per kilogram.

C2.3.7 Instructions for Section 4: Additional Information

In section 4, the user enters additional information needed to generate the trial batch experimental plan. This information includes the number of center points to be run and a random number seed. Steps for entering this information (see figure C-7) are as follows:

The fourth step is to provide additional information needed to generate the experimental plan.

Please select the number of center points to use in this study and enter a random number seed (less than zero) to randomize the run order.

Select number of center points to run: [3]

Random number seed less than zero: [-3034]

The final step is to enter a filename (no extension) to store the mixture proportion information. This should be the same name that you used when specifying the response variables earlier.

Filename (no extension, **eight** characters maximum): [mix001]

[Submit form for response] [Reset all values to defaults]

Return to top of page

Figure C-7. Fourth section of "Mixture Factors..." form (additional information section)

- **Enter the number of center points** to use in the experiment, using the pulldown menu. Center points are experimental runs in which all factors are set at the midpoints of their ranges. The coded values for the low and high settings are –1 and +1, respectively. The coded values for the center points are zero. Center point mixes are replicated to estimate pure error and also may be used as control mixes to assess variation over time. It is a good idea to run at least 3 center points to assess this variation.

- **Enter a random number seed** (any number less than zero). This is used to generate a random run order for the experiment.

- **Enter the filename** in which to store the information. This name should be the same as that entered in "Specify Responses." Again, the filename is entered without an extension (COST adds the appropriate extensions as necessary).

After entering the filename, the user may click on "Submit" to submit the information to COST and generate the experimental plan, or the user may click "Reset" to set all values back to their defaults (all information entered will be lost).

When "Submit" is clicked, COST processes the input and generates an experimental plan, which is displayed on the screen. The user should print this plan using the "PRINT" command in the browser. An example of a portion of an experimental plan generated by COST is shown in figure C-8.

Mixture Proportions for datafile– mjs5t1

Run_number	Mix_number	Water (kg/m³)	Cement (kg/m³)	Coarse_aggregate (kg/m³)	Fine_aggregate (kg/m³)	Silica_fume (kg/m³)	HRWRA (kg/m³)	Cost
1	27	148.79	390.64	1147.50	743.33	41.01	7.03	93.71
2	10	177.81	427.45	1080.00	675.75	58.29	9.23	110.59
3	14	154.27	367.79	1215.00	675.75	50.15	5.30	99.56
4	2	163.96	469.37	1080.00	675.75	64.00	6.76	118.52
5	12	152.40	367.79	1080.00	810.90	50.15	5.30	99.57
6	5	146.26	417.88	1215.00	675.75	31.45	6.02	87.31
7	1	168.25	485.41	1080.00	675.75	36.54	10.48	96.39
8	15	131.52	317.29	1215.00	810.90	23.88	4.57	73.97
9	13	158.04	379.25	1215.00	675.75	28.55	8.19	82.06
10	30	148.79	390.64	1147.50	743.33	41.01	7.03	93.71
11	7	118.74	346.72	1215.00	810.90	26.10	7.49	78.89
12	16	125.56	305.32	1215.00	810.90	41.64	6.59	89.03
13	4	137.14	400.64	1080.00	810.90	54.63	8.65	106.84
14	9	186.15	444.21	1080.00	675.75	33.44	6.40	89.51
15	11	156.17	379.25	1080.00	810.90	28.55	8.19	82.06
16	3	144.40	417.88	1080.00	810.90	31.45	6.02	87.31
17	6	139.00	400.64	1215.00	675.75	54.63	8.65	106.84
18	8	115.67	335.26	1215.00	810.90	45.72	4.83	94.69

Figure C-8. Portion of an experimental plan generated by COST

The columns in the printed table shown above correspond to the run number (the order in which the mixtures should be prepared), the mixture number (the mixture number according to standard experiment design tables), mixture proportions in terms of the mass of each component per cubic meter of concrete, and an estimated cost for each mixture based on the individual material costs provided by the user.

If the plan is not printed immediately, it can be viewed and printed at a later time by selecting "View Expt Plan" from the main menu.

C2.4 Step 3—Run Trial Batches

The next step after generating an experimental plan is to actually perform the experiment. The experiment in this case is a set of trial batches from which specimens will be fabricated and tested for the responses and mixture components specified in steps 1 and 2. Before running the experiment, steps 1 and 2 must be complete, and the user should have a printed copy of the experimental plan containing the mixture proportions for the set of trial batches.

When "Run Trial Batches" is selected from the main menu, the screen shown in figure C-9 appears. This screen does not require any input; rather, it provides instructions and guidelines for running the trial batches. These guidelines are also provided below.

Run the Experiment (Trial Batches)

The next step after generating an experimental design is to actually perform the experiment. The experiment in this case is a set of trial batches from which specimens will be fabricated and tested for the responses and mixture components specified in Steps 1 and 2. At this point you should have completed Steps 1 and 2 and obtained a printed copy of the experimental plan (mix proportions for the set of trial batches). If you have not done so, click on the appropriate selections on the left hand side bar.

If you have completed Steps 1 and 2 but have not printed a copy of the experimental plan, click here to view or print a copy of the experimental plan.

Step 3 is the most time-consuming of the 6-step procedure in that you must physically run the experimental plan and collect data on the performance variables of interest to you. Running the experiment includes the following tasks:

- ordering and preparing the materials needed for the experiment
- ensuring that equipment is available and ready for use
- coordinating personnel
- batching, fabricating, testing and recording data (running the experiment)

IMPORTANT! If you are ready to run the experiment, please read the following sections which describe important considerations to keep in mind while performing the experiment

1. Nuisance Factors and Run Sequence Randomization
2. Running the Experiment

---

1. Nuisance Factors and Run Sequence Randomization

Your experiment has three types of factors:

- Major factors (variable factors)
- Fixed factors
- Nuisance factors

The primary goal of your experiment is to determine optimal settings of the *major factors* that were selected as variable factors in Step 1. You may have also designated some *fixed factors* to be held constant throughout the experiment.

Figure C-9. "Run Trial Batches" screen

C2.4.1 Guidelines for Running Trial Batches

Running the experiment is the most time-consuming task because it involves physically running the experimental plan and collecting data on the performance variables of interest. Running the experiment includes the following tasks:

- Ordering and preparing the materials needed for the experiment.
- Ensuring that equipment is available and ready for use.
- Coordinating personnel.
- Batching, fabricating, testing, and recording data (running the experiment).

The following sections describe important considerations to keep in mind while performing the experiment.

C2.4.2 Nuisance Factors and Run Sequence Randomization

There are three types of factors that affect the responses in an experiment:

- Variable factors.
- Fixed factors.
- Nuisance factors.

The primary goal of the experiment is to determine optimal settings of the variable factors specified in step 1. These are the major factors of interest. Depending on the objective, some fixed factors may have also been designated. These are less important factors that are held constant throughout the experiment.

The variable factors and fixed factors are controlled in the experiment. However, in addition to these, there are other factors that are not controlled in the experiment but which could possibly affect the experimental results. These are called nuisance factors. It is often assumed that these nuisance factors do not, or should not, have any effect, but in reality they may have an effect. Nuisance factors may include the following:

- Mid-experiment changes in instruments, equipment, environmental conditions, (temperature, pressure, humidity, etc.), measuring devices.
- Test procedures/protocols.
- Day of week.
- Time of day.
- Operators.

Nuisance factors may affect the measured test results, which would in turn affect the data analysis, and ultimately the final conclusions (i.e., the estimated values for the optimal mixture proportions).

Run sequence randomization is used to minimize the effect of nuisance factors. Experiment designs are usually generated in a "standard order" based on the settings of the factors. This order (used by COST in the data analysis) is indicated by the "mixture number" column (column 2) in the experimental plan generated by COST (figure C-8). Run sequence randomization is the general experiment design technique in which random numbers are assigned to each of the specified runs in the experiment, and these random numbers determine the order in which the experiment is to be run (the "run order" or "run sequence"). The experimental plan generated by COST is printed in run order—the first column of the experimental plan, labeled "run number," is the run order to be used for the experiment (figure C-8).

It is very important to follow the run sequence in order to minimize possible error in the experimental results caused by known or unknown nuisance factors in the experiment.

C2.4.3 Running the Experiment

The quality and accuracy of the final mixture proportion settings will depend very much on the care taken in carrying out the experiment. The following is a list of recommended practices:

- Attention to detail, consistency and proper execution in batching, mixing, fabricating, curing, testing, and recording results are essential.

- For each trial batch, use several (preferably 3 or more) specimens for each test.

- The experimental plan contains 3 or 5 center point runs. These are replicates (repeats of batches using the same settings) which can be used during the experiment as control mixes. Scheduling to allow for one control mixture per week is recommended—in this way significant week-to-week variation can be detected.

- If possible, the same operator should perform the same tasks throughout the experiment.

- Mistakes will inevitably occur even in the best laboratories, and it is important to acknowledge this and to be prepared to repeat a batch if it is suspected that an error has occurred.

C2.5 Step 4—Input Results

This section describes how to input experimental results into the COST program for analysis. The following instructions assume that steps 1, 2, and 3 have been successfully completed. Within this step, you may perform the following tasks:

- Change cost information (optional).
- review the experimental plan (optional).
- enter or edit the experimental results (data) for analysis (**required**).

Instructions for each of these tasks are provided below.

C2.5.1 Instructions for Changing Cost Information

Before entering the test results, you may optionally change the costs of the raw materials, if you have updated information since the project began. *Please note that these updates should be made before entering in the data (test results) as described below; otherwise, the new costs will not be in effect during the analysis phase.* To do so, click on the link "Update cost information." You will see a box with the caption "Datafile name". Enter the name of your datafile (no extension) in the box, and press the "Submit" button. A form entitled "COST Input Form: Update Material Costs for 'DATAFILE'" will appear. Make any necessary changes to the material costs and press "Submit" to save the changes.

If you make a mistake and would like to reset all costs to their default values, press "Reset," before pressing the "Submit" button. If you decide not to change the costs, simply press the back button on your browser to return to the previous page, or select any entry from the blue menu sidebar.

C2.5.2 Instructions for Entering/Editing Data

When you are ready to enter your data, click on "Enter or edit data in chronological (run) order." You will then see a screen entitled "COST Input Form: Testing Results (Project Filename)." Enter the project filename (with no extension) and press "Submit."

The next screen will be "COST Input Form: Test Results for 'DATAFILE.'" The first part of this form, as shown in figure C-10, allows you to make changes to the response information that you entered in step 1 (instructions are the same as for step 1 described previously). If you do not have any changes to make in the response information, simply scroll down to the second part of the form.

The second part of the form is for entry (or editing) of the experimental results, or data. The last two lines in the figure C-10 show two rows of entries for the experimental test results. The first column shows the run order for the experiment, and the second column shows the mixture number (these should correspond to the run and mixture numbers in your experimental plan). The third column is "Cost" (the first response).

Please supply the following information for your tested mixtures

Response:		Cost	Slump	28-day_Str	1-day_Str	RCT
Units		$_(USD)	mm	MPa	MPa	Coulombs
Lower limit		50.00	50.00	50.00	20.00	100.00
Upper limit		99.00	100.00	80.00	50.00	1000.00
Result weight		1.00	1.00	1.00	1.00	1.00
Weight function type		Minimum	Target	Maximum	Maximum	Minimum is
Run number	Mix Number					
1	27	93.72	73.00	58.50	16.30	286.00
2	10	110.59	102.00	60.40	16.47	296.00

Figure C-10. Data entry form for the COST system

IMPORTANT: Because the total cost of each mixture is calculated from the individual materials costs entered in step 1, the third column contains nonzero entries that should not be changed.

The **responses requiring data entry** start in the fourth column (one column per response).

- **If you are entering results for the first time**, these columns will contain zeros. Enter the appropriate results in these columns for each mixture.

- **If you are editing a file you already created**, these columns will contain nonzero values. Perform any necessary editing.

IMPORTANT: As you enter or edit your data, please check the input as you go for typographical errors and to make sure that the results are entered in the correct columns and rows.

It should be noted that some of the input values shown in figure C-10 are outside of the acceptable range specified by the lower and upper limits, as will most likely be the case for any real experiment.

When data entry is complete, you may use the "PRINT" button on your browser to print the input form.

IMPORTANT: It is highly recommended that you check the printed form for accuracy, and edit the information if necessary (to edit, simply follow the instructions in this section).

C2.6 Step 5—Analyze Data

The next step after entering the data is to analyze the results, with the ultimate goal of determining optimal mixture proportions. The analysis techniques employed by COST consist of both graphical analysis and numerical analysis (modeling). The analysis is broken down into 10 tasks, which are described in detail below.

C2.6.1 Instructions for Changing Response Information

Before analyzing the data, COST gives the user the option of changing response variable limits, weights, and function types. To do so, click on "Change response variable limits, weights, and function types." You will then be prompted for the filename. After entering the filename, press "Submit" and follow the instructions in the section "Step 1—Specify Responses."

C2.6.2 Analysis Tasks

The analysis tasks are listed by the purpose of the task followed by the statistical tool used to perform the task, as shown in figure C-11. For example, the purpose of task 2 is to "Assess the Balance of the Design," and the tool used is "Counts Plot Matrix of Factors." An example and explanation of each task and tool is provided below. The output of each task is a GIF file that is generated by DATAPLOT. The GIF file contains tabular output, graphical output, or a combination of both.

COST provides both graphical and numerical analysis of your data. The graphical analysis includes various types of plots which are described below. The numerical analysis includes fitting an empirical model to the data, verifying adequacy of the model, and numerical optimization.

Performing the Analysis - Task by Task

Task 1: Characterize the Response Variables
Tool: Summary Statistics

Task 2: Assess the Balance of the Design
Tool: Counts Plot Matrix of Factors

Task 3: Assess Optimality of Design Points for All Responses Jointly
Tool: Matrix of Counts-in-admissible-region plots

Task 4: Assess Optimality of Design Points for All 4 Responses Jointly
Tool: Matrix of Percentage-in-admissible-region plots

Task 5: Determine Interrelationships between Response Variables
A. Tool: Scatter Plot Matrix of Response Variables
B. Tool: Scatter Plot Matrix of Response Variables versus Factors

Task 6: Assess Relationship Between Response Variables & Factors
Tool: Mean Plots of Response Variables versus Factors

Task 7: Determine Optimal Settings for Each Factor
A. Tool: Best Settings Based on Mean Values
B. Tool: Best Settings Based on Individual Runs

Task 8: Model Fitting and Verification
A. Tool: Model Fitting Tool

Task 9: Numerical Optimization
A. Tool: Best Settings - Maximization of Total Score Fitted Function

Task 10: Response Prediction
Tool: Response Prediction Tool

Figure C-11. Analysis menu showing individual analysis tasks

C2.6.2.1 Task 1: Characterize the Response Variables

This task provides a quantitative summary of the data for each response. The result of this task is a table of descriptive statistics such as mean, range, and standard deviation for each response. An example is provided below (figure C-12).

TASK 1: SUMMARIZE THE 5 RESPONSE VARIABLES
DATA FILE = MJS98E
STAT TOOL: SUMMARY STATISTICS

	Y1 COST	Y2 SLUMP	Y3 ?-DAY_STR	Y4 28-DAY_STR	Y5 RCT	TS TOTAL SCORE
PROJECT GOAL	MIN	TARGET	MAX	MAX	MIN	MAX
SPEC MIN	50	2	2860	7150	100	0.5
SPEC MAX	99	4	7150	11440	1000	1
DATA COUNT	31	31	31	31	31	31
DATA # IN SPEC	3	15	11	31	31	26
DATA % IN SPEC	10%	48%	35%	100%	100%	84%
DATA MIN	90.56	0.5	1867	7301	160	0.41
DATA MEAN	107.78	2.55	2704.61	8249.65	319.06	0.59
DATA MEDIAN	107.71	2.5	2672	8213	286	0.61
DATA MAX	124.87	6	3826	9782	705	0.74
DATA RANGE	34.31	5.5	1959	2481	545	0.33
DATA SD	8.1	1.6	430.83	619.95	124.53	0.08
DATA REL. SD	8%	63%	16%	8%	39%	14%

Figure C-12. Summary statistics table (output of analysis task 1)

The summary statistics provided for each response and the total score (TS) are described in table C-3 (next page).

Table C-3. Description of summary statistics provided in analysis task 1

Statistic	Description
PROJECT GOAL	optimization goal for response
SPEC MIN	minimum value specified by user
SPEC MAX	maximum value specified by user
DATA COUNT	number of data points read(runs)
DATA # IN SPEC	number of runs with response meeting spec
DATA % IN SPEC	percentage of runs with response meeting spec
DATA MIN	minimum response value
DATA MEAN	mean response value
DATA MEDIAN	median response value
DATA MAX	maximum response value
DATA RANGE	range of response values (max - min)
DATA SD	sample standard deviation
DATA REL. SD	SSD relative to mean (coefficient of variation)

C2.6.2.2 Task 2: Assess the Balance of the Design

This task is a check to make sure that the design is balanced. The result of this task is a plot similar to figure C-13. Figure C-13 shows a matrix of plots showing the number of design points (experimental runs) at each setting for all combinations of two factors. For example, the highlighted box in figure C-13 shows the number of design points for the factors X2 and X3 (fine aggregate and coarse aggregate). There are nine numbers in this box, representing different settings of the factors. The lower left number indicates that there are 4 design points that have the setting "-1, -1" (in coded values) for fine aggregate and coarse aggregate. For this design every set of two factors has the same experimental layout (the sets of nine numbers in each box are the same). For any design generated by COST, this will always be the case. The percentage in the upper left corner indicates the correlation coefficient. Ideally, this will be zero. For any design generated by COST, the correlation coefficient will be zero for all sets of factors, indicating a balanced design.

TASK 2: ASSESS THE QUALITY OF THE EXPERIMENT DESIGN MJS98R

TOTAL NUMBER OF DESIGN POINTS (RUNS) = 31

STAT TOOL: COUNTS PLOT MATRIX OF FACTORS

CHARACTER = NUMBER OF DESIGN POINT RUNS

LEGEND = CORR. COEFF. (BEST CC = 0% WORST CC = +/-100%)

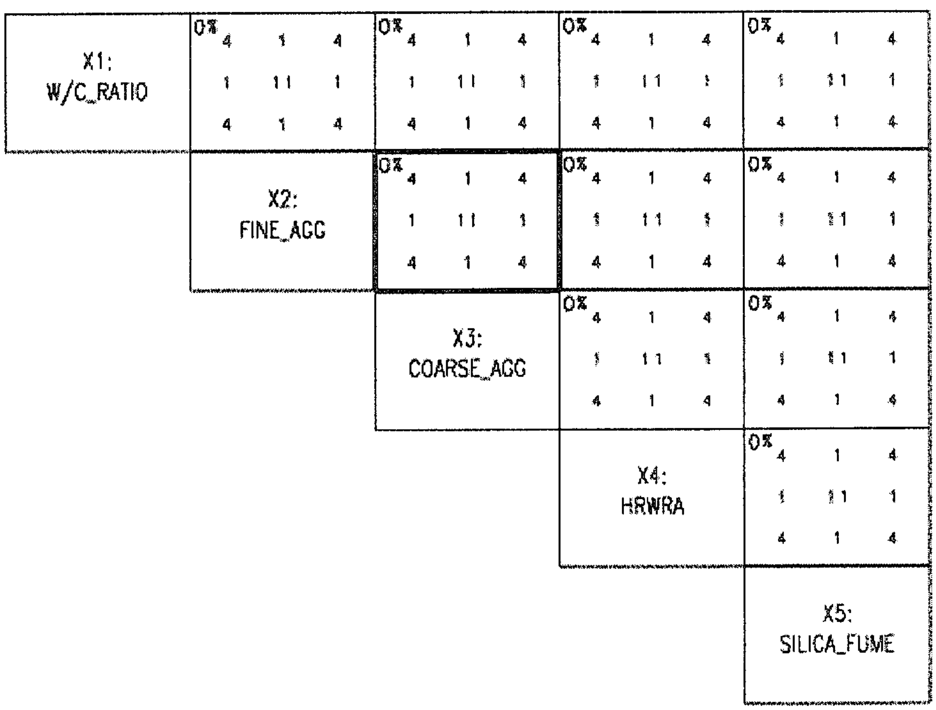


Figure C-13. Output of analysis task 2 (counts plot matrix of factors)

C2.6.2.3 *Task 3: Assess Optimality of Design Points for All Responses Jointly*

The purpose of task 3 is to see how all the responses compare to the specifications for each design point. Figure C-14 shows the output, which is a matrix of plots comparing each combination of two factors. In each large box there are nine smaller boxes, corresponding to the nine possible design settings for two factors. In each smaller box there will be between one and five numbers, depending on the number of responses being investigated. In the example below, there are five responses, and thus five numbers. The legend at the lower left of the plot indicates which number in the small box corresponds to which response (Y1, Y2, Y3, Y4, Y5). In the example below, the large box for X2 and X3 is highlighted, and the small box corresponding to settings of X2 = 0, X3 = 0 is highlighted. The numbers in the small box indicate that for these settings of X2 and X3, there was 1 response for Y1 that was within the acceptable region, there were 7 for Y2, 2 for Y3, 11 for Y4, and 11 for Y5. This information allows the user to assess how well the ranges selected for the factors allow him to meet the desired specifications. For Y1 and Y3, only a few responses met the specification. Therefore, for this set of mixture proportions, it may be difficult to optimize these responses. A new set of acceptance criteria could be defined, or different ranges for the mixture proportion factors may be needed. Other analysis tasks will give the user a sense of which direction the factors must be shifted.

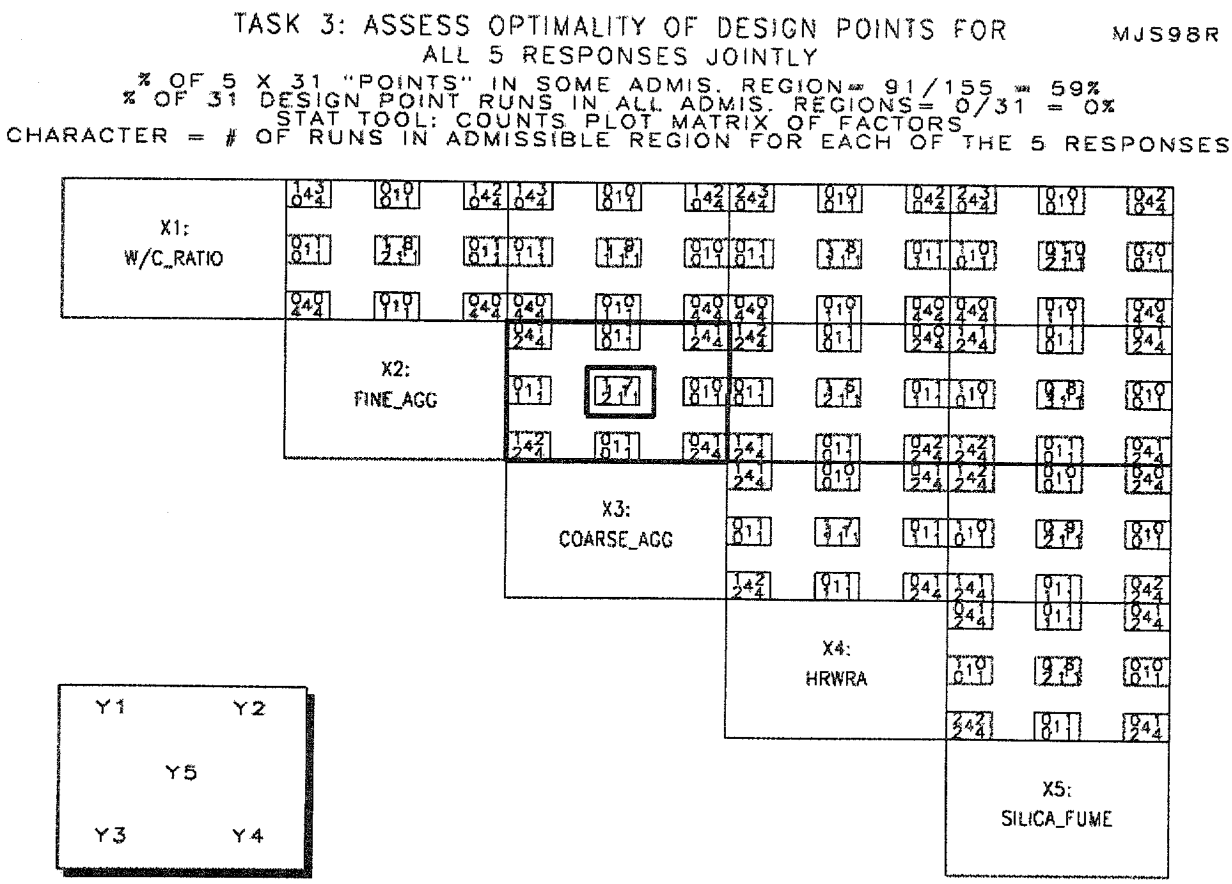


Figure C-14. Output of analysis task 3 (counts plot matrix of factors)

C2.6.2.4 Task 4: Assess Optimality of Design Points for All Responses Jointly

Task 4 is similar to task 3 in assessing optimality of design points. For each combination of two variable settings (e.g., X2 = 0, X3 = 0), the percentage of runs falling in at least one admissible region (for all responses taken together) is shown (see figure C-15). The overall percentage for all the runs is given in the first text line below the title. In this case, it is 59 percent. The overall percentage for the number of design points meeting all "n" (in this case, 5) acceptance criteria for responses is indicated on the second line below the title. In this case, it is zero. The gray squares over the numbers in the boxes indicate the highest percentage in each box, and the triangles indicate the lowest percentage in the box. This gives a quick visual cue to the settings that are best in meeting the acceptance criteria.

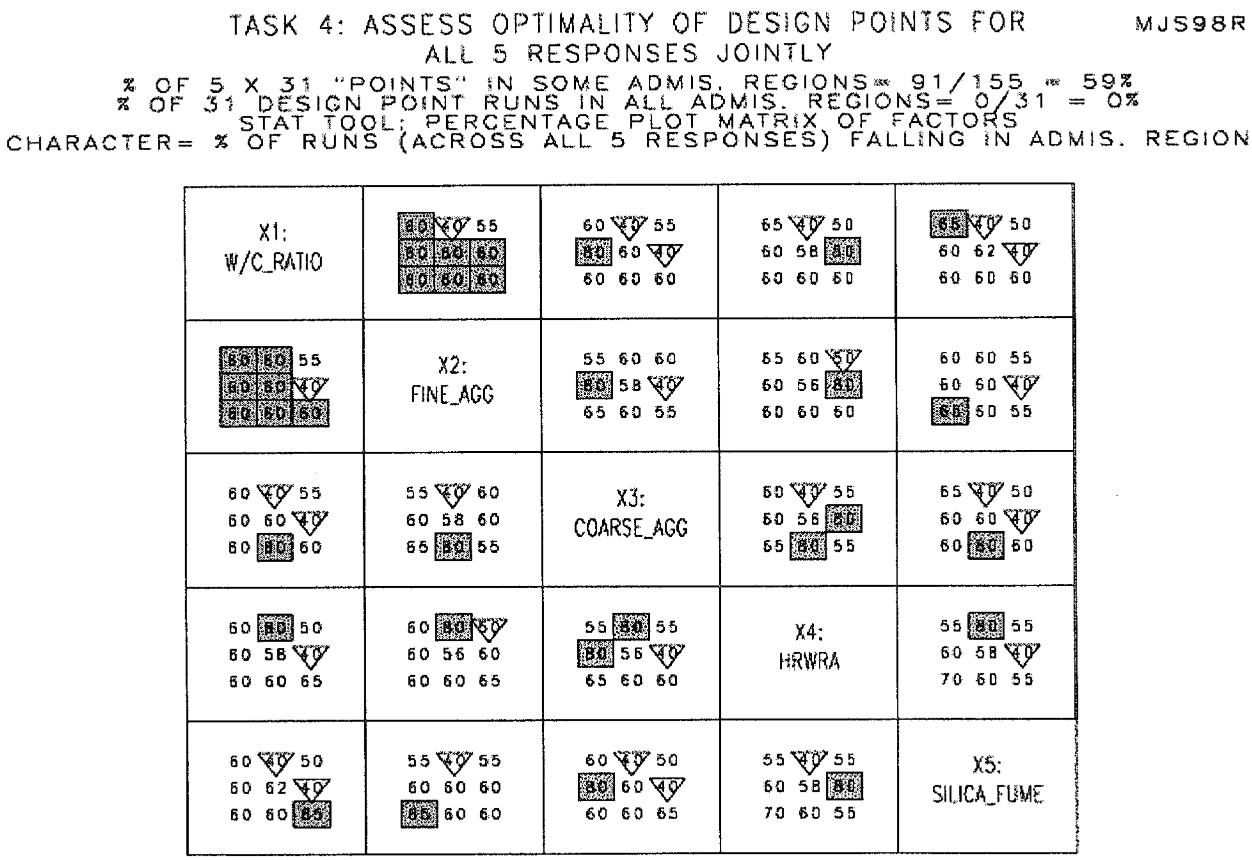


Figure C-15. Output of analysis task 4

C2.6.2.5 *Task 5A: Determine Interrelationships between Response Variables*

Figure C-16 shows a matrix of scatterplots showing data for each combination of two response variables (RVs). The admissible region for each **pair** of RVs is indicated as a gray box surrounded by dashed lines. These plots give a sense of relationships between responses and also a sense of how many points fall in the admissible region (as defined by the performance criteria set by the user) for each pair of responses. The numbers in the upper left corner of each box (e.g., 2/31 = 6 percent) indicate the number of responses falling in the admissible region. The large gray shaded box at the bottom left of the entire plot shows the relative ease or difficulty of meeting the performance criteria (i.e., falling within the admissible region) for single responses and for pairs of responses.

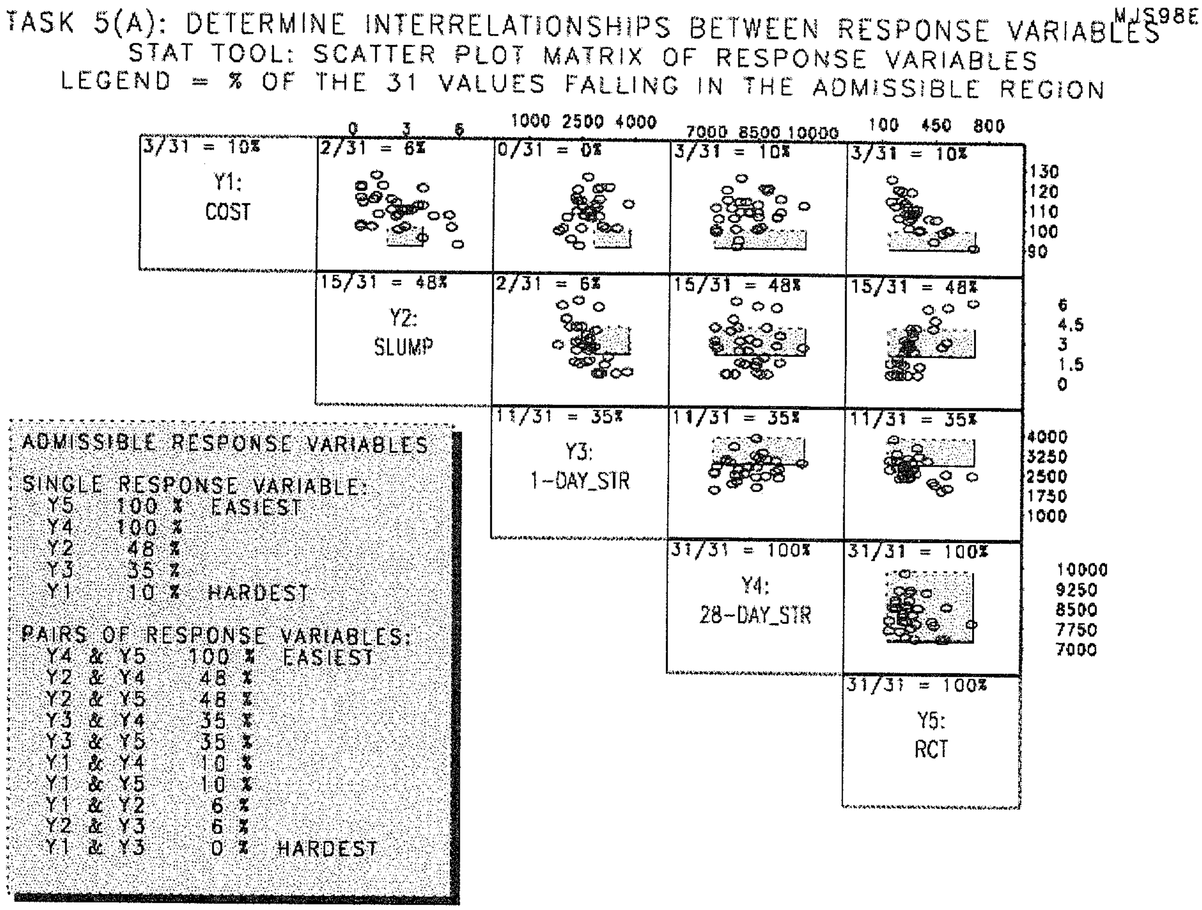


Figure C-16. Output of analysis task 5A

C2.6.2.6 Task 5B: Interrelationships between Response Variables and Factors

The output for this task (shown in figure C-17) shows the relationship between responses and factors. In each plot, the response values (Y axis) are shown for each factor level (X axis). The correlation coefficient (indicating the strength of the linear relationship between Y and X) is shown in the upper left corner of each plot. The stronger the linear relationship, the closer this value will be to 1 or –1 (depending on the slope). Examining these plots allows the user to assess which factors are important (controlling) for each response. The gray shaded boxes at the bottom of the plot summarize the control factors (left box, percentage indicates correlation coefficient) and the "weak" factors (right box).

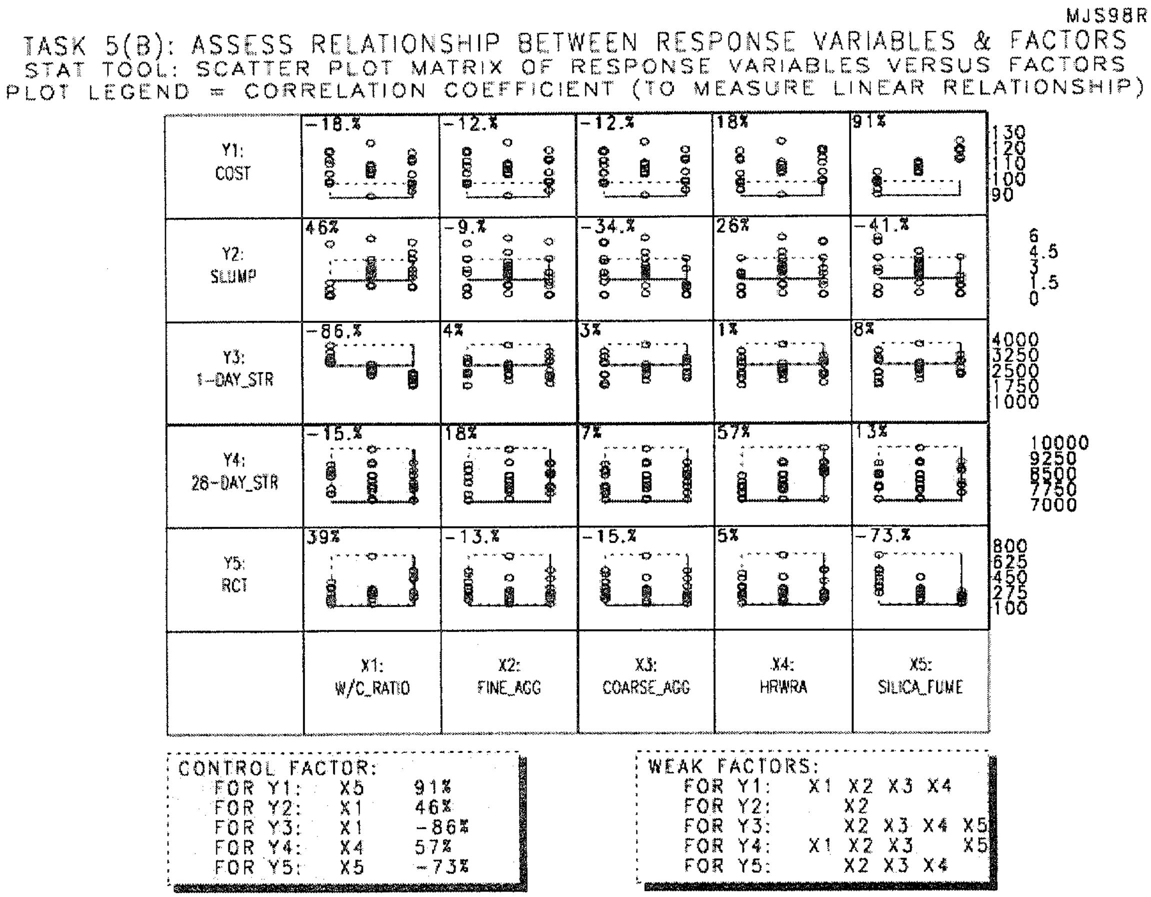


Figure C-17. Output of analysis task 5B

C2.6.2.7 Task 6: Assess Relationship between Response Variables and Factors

This task provides an assessment of the relationship between responses and factors by examining plots of the mean (average) values of the responses at each factor level. Figure C-18 shows the output for this task. For each response, there is a plot of the mean values at each level of each factor. The gray shaded boxes indicate the admissible region for each response. Influential factors are those that have a definite slope (for example, silica fume for response Y1, cost, or w/c ratio for Y3, 1-day strength). The steeper the slope, the more important the factor. A flat line (or nearly flat) indicates little effect of the factor (for example, fine aggregate for Y5, RCT).

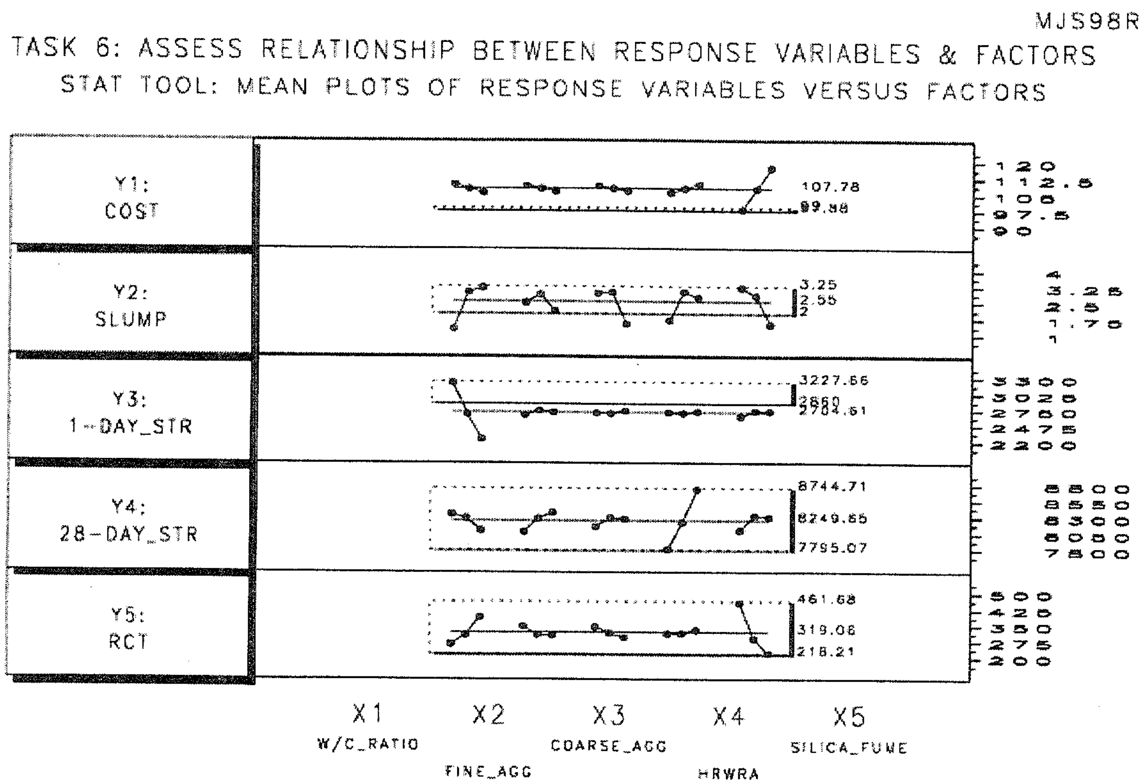


Figure C-18. Output of analysis task 6

C2.6.2.8 Task 7A: Best Settings for Each Factor Based on Means

This task provides a graphical means of selecting best factor settings based on mean (average) values of "scoring functions" calculated for each response separately as well as a total score function (TS). The total score is a weighted linear combination of scores calculated for each response (the weight given to each response is defined in "Step 1—Specify Responses," as the result weight, a value ranging from zero to 1). Figure C-19 shows the output from this task.

The best settings (as coded values) are shown in parentheses on the right side of each plot. The best setting based on total score are shown in the gray box at the bottom of the plot, in both coded and actual units. As in task 6, a steep slope indicates a large influence of a particular factor on the score, while a flat slope indicates little or no influence.

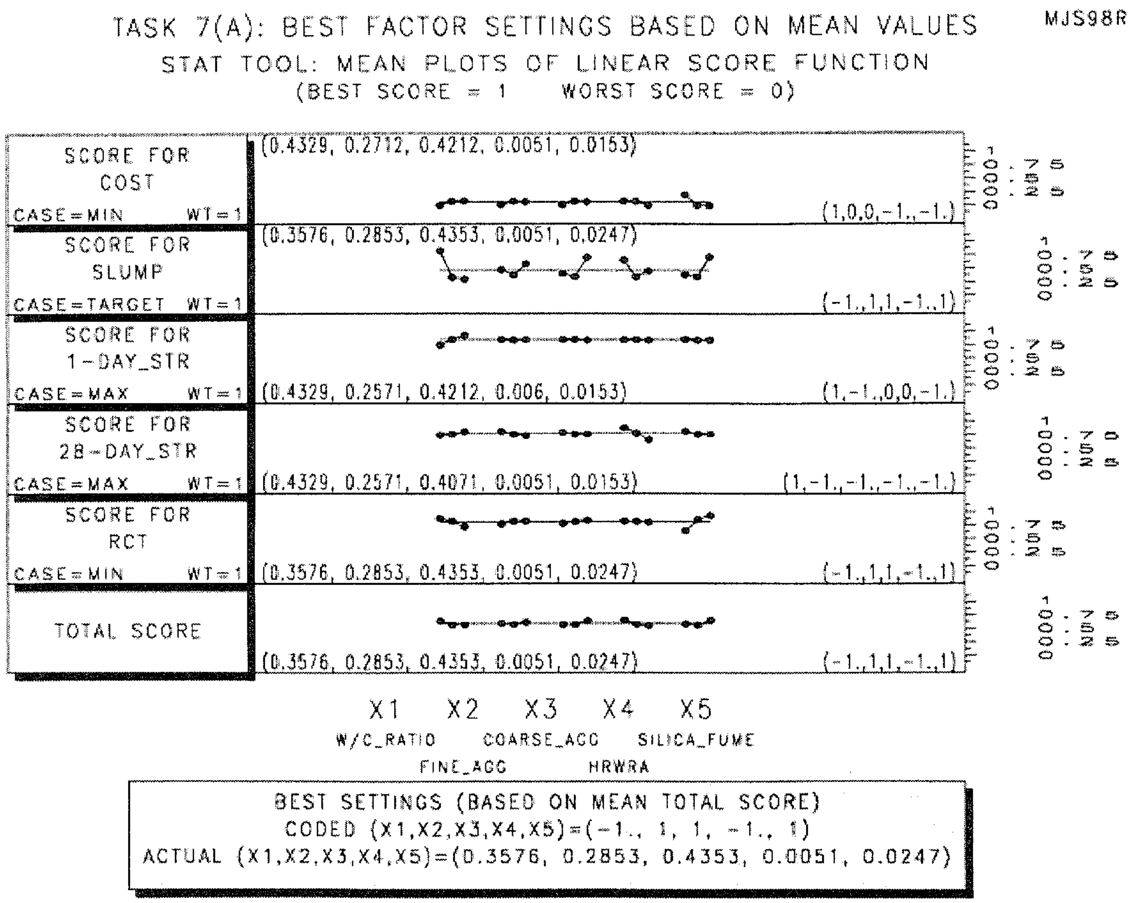


Figure C-19. Output of analysis task 7A

C2.6.2.9 Task 7B: Best Factors Based on Individual Runs

This task produces a plot (figure C-20) showing the best settings for total score (weighted linear combination of scores for individual responses) based on individual runs. The total scores for each run are calculated, sorted (lowest to highest) and plotted along the X axis. The Y axis is used to differentiate between the individual runs. Each run is indicated by its number in the experimental plan, and the coded values of each factor are provided in parentheses on the right. These values are staggered for readability. The topmost number has the highest total score.

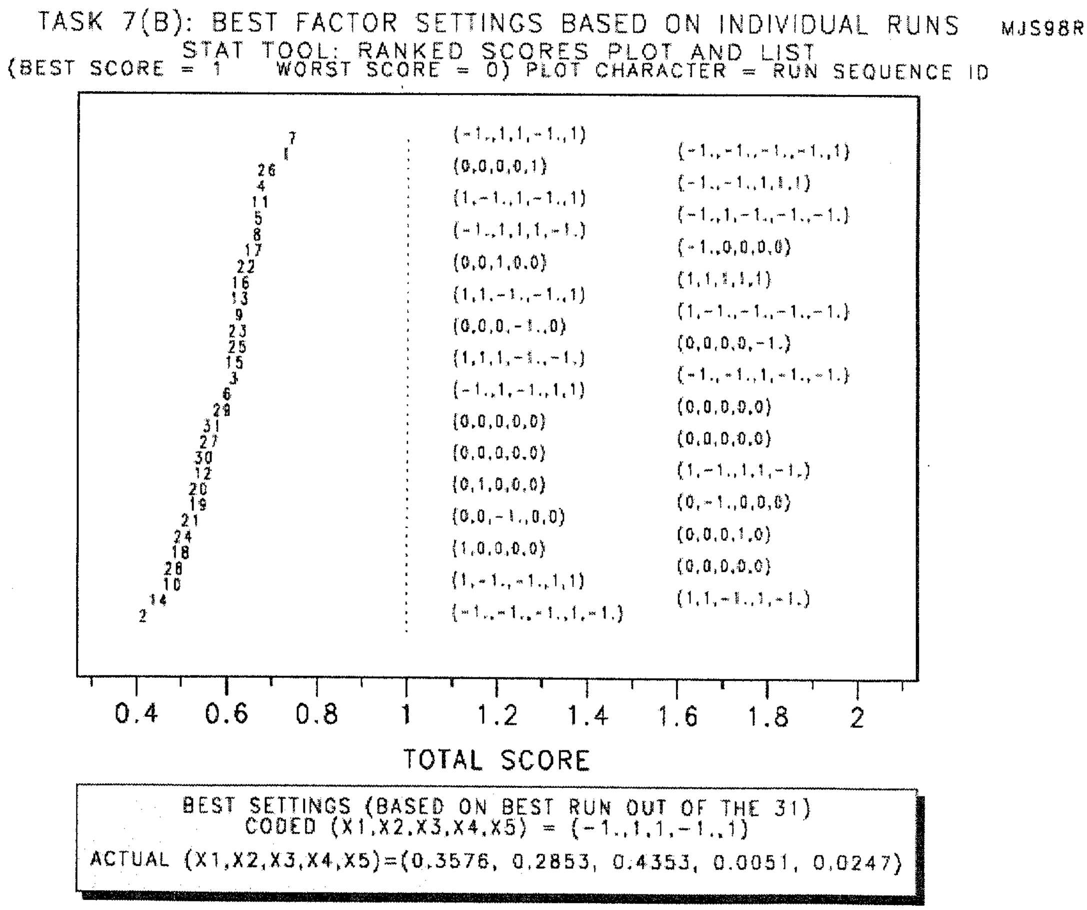


Figure C-20. Output of analysis task 7B

C2.6.2.10 Task 8: Model Fitting and Verifications

In this task, an empirical mathematical model is fitted to the data for each response, and to the total score, using the standard regression methods (least squares). A full quadratic model is fit initially, and then reduced by eliminating terms with significance level less than 0.05. When the task is selected, the response to be fitted is selected using a pull-down menu. In addition to the response variables (up to five), a model may also be fitted to total score. For a complete analysis of all responses, task 8 must be thus executed multiple times, once for total score and once for each response variable. Output similar to figure C-21 is produced for the each selected response variable. The output provides a plot for the response as a function of each factor, showing all response data for the coded values of each factor. These plots may indicate trends (see for example, the plot for silica fume in figure C-21, which indicates a downward trend in RCT test results with increasing silica fume). In addition to the plots, a summary box of the important terms in the model is provided to the right of the second row of plots, and the actual model is printed below the plots. The model is in terms of CODED values (the model can be translated to actual factor values). The model can be used to predict the response values for settings other than those used in the experiment (but within the experimental space)—a calculator for doing this is provided in task 10.

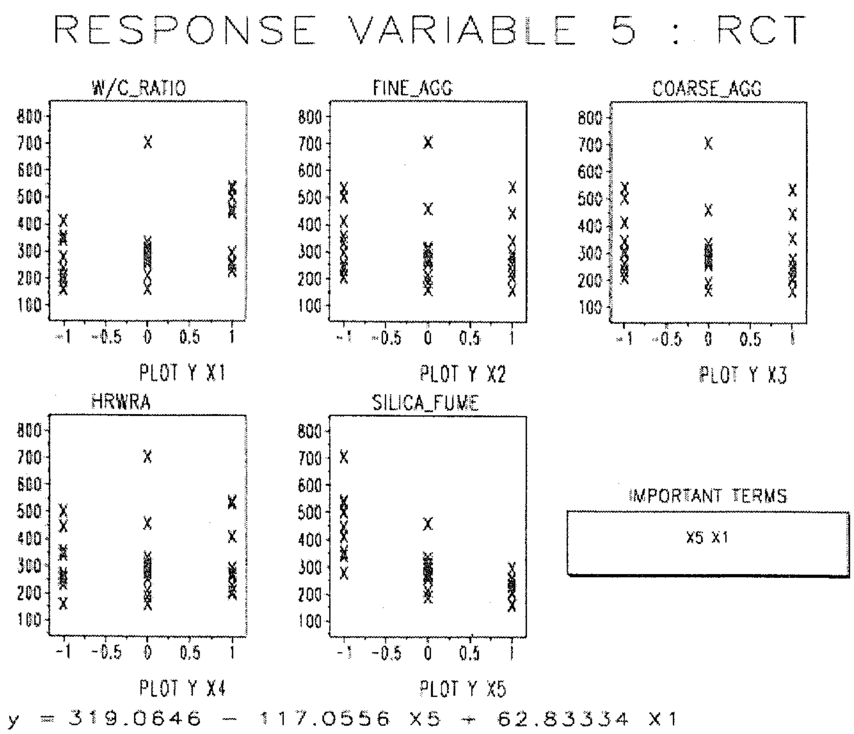


Figure C-21. Output of analysis task 8 (for response RCT)

C2.6.2.11 Task 9: Numerical Optimization

This task uses numerical optimization techniques to identify the optimal settings for total score, over the entire experimental space. This optimization is performed during the model fitting for total cost in task 8, so when task 9 is executed, the COST system simply returns a table indicating the best settings as determined by the numerical optimization, as shown in figure C-22.

Results for Mixture mjs98e

Optimization Determined by Numerical Optimization

Units are the same as those used in the specify mixtures form previously

Aggregates are in terms of volume or mass fraction (as previously selected by user)

Mineral admixtures are in terms of percent cement mass replacement

Chemical admixtures are in terms of liters per kg of cement

Variable	Optimum setting
w/c_ratio	0.3576
fine_agg	0.2712
coarse_agg	0.4071
HRWRA	0.0051
Silica_fume	0.0228

Above optimization performed by DATAPLOT

Figure C-22. Output of analysis task 9

C2.6.2.12 Task 10: Response Prediction

As shown in figure C-23, this task provides a calculator for predicting response values using the models from task 8. The user enters values for each factor (in terms of actual values) and the program calculates the responses and the total score. Calculations can be performed for up to 10 different combinations of factors.

Prediction of Responses

Fill in the x-values under the columns with black titles and the calculated responses will appear under the magenta headings. **Press the Update Calculations button to calculate for the shown initial values.**

Update calculations

w/c_ratio	fine_agg	coarse_agg	HRWRA	Silica_fume	Total_score	Cost	Slump	1-day_Str	28-day_Str	RCT
0.3576	0.2571	0.4071	0.0051	0.0247	.6199999	113.1713	1.613874	2859.057	7962.552	241.5399
0.3576	0.2571	0.4071	0.0051	0.0247	.6199999	113.1713	1.613874	2859.057	7962.552	241.5399
0.3576	0.2571	0.4071	0.0051	0.0247	.6199999	113.1713	1.613874	2859.057	7962.552	241.5399
0.3576	0.2571	0.4071	0.0051	0.0247	.6199999	113.1713	1.613874	2859.057	7962.552	241.5399
0.3576	0.2571	0.4071	0.0051	0.0247	.6199999	113.1713	1.613874	2859.057	7962.552	241.5399
0.3576	0.2571	0.4071	0.0051	0.0247	.6199999	113.1713	1.613874	2859.057	7962.552	241.5399
0.3576	0.2571	0.4071	0.0051	0.0247	.6199999	113.1713	1.613874	2859.057	7962.552	241.5399
0.3576	0.2571	0.4071	0.0051	0.0247	.6199999	113.1713	1.613874	2859.057	7962.552	241.5399
0.3576	0.2571	0.4071	0.0051	0.0247	.6199999	113.1713	1.613874	2859.057	7962.552	241.5399
0.3576	0.2571	0.4071	0.0051	0.0247	.6199999	113.1713	1.613874	2859.057	7962.552	241.5399

Figure C-23. Calculator for predicting responses based on models

C2.7 Step 6—Summarize Analysis

This step simply returns a table summarizing the three different optimum settings (from analysis tasks 7A, 7B, and 9) determined by the COST system, as shown in figure C-24.

Summary of Results for Mixture mjs98e

Variables examined:

w/c_ratio fine_agg coarse_agg HRWRA Silica_fume

Responses evaluated:

Cost Slump 1-day_Str 28-day_Str RCT

Optimum Settings

Units are the same as those used in the specify mixtures form previously

Aggregates are in terms of volume or mass fraction (as previously selected by user)

Mineral admixtures are in terms of percent cement mass replacement

Chemical admixtures are in terms of liters per kg of cement

Variable	Mean Values Optimum setting	Individual Runs Optimum setting	Numerical Optimization Optimum setting
w/c_ratio	0.3200	0.3576	0.3576
fine_agg	0.2853	0.2853	0.2712
coarse_agg	0.4353	0.4353	0.4071
HRWRA	0.0051	0.0051	0.0051
Silica_fume	0.0294	0.0247	0.0228

Figure C-24. Example summary returned by the COST system

SECTION 3
References

1. Box, G.E.P., Hunter, W.G., and J.S. Hunter, *Statistics for Experimenters*. New York, John Wiley & Sons, 1978.

2. Myers, R.H. and D.C. Montgomery, *Response Surface Methodology: Process and Product Optimization Using Designed Experiments*. New York, John Wiley & Sons, 1995.

3. Simon, M.J., Lagergren, E.S, and L.G. Wathne, "Optimizing High-Performance Concrete Mixtures Using Statistical Response Surface Methods." In *Proceedings of the 5th International Symposium on Utilization of High-Strength/High-Performance Concrete*. Norwegian Concrete Association, Oslo, Norway, June, 1999, pp. 1311-1321.

4. Heckert, A., and J.J. Filliben, DATAPLOT Reference Manual Volume I: Commands, National Institute of Standards and Technology, 1999.

HRD/-12/09-03/976/E